



## A Windows program for calculation and classification of epidote-supergroup minerals

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### ABSTRACT

A Windows program, called WinEpcas, has been developed to calculate and classify wet-chemical and electron-microprobe epidote-supergroup mineral analyses based on the Commission on New Minerals and Mineral Names (CNMMN) of the International Mineralogical Association (IMA-06) nomenclature scheme. WinEpcas enables the user to enter epidote-supergroup mineral analyses in the *Data Entry Screen* as well as loading previously typed Microsoft® Excel files. The program allows the users to type 43 variables of epidote-supergroup mineral analyses in program's data edit section. Mineral analyses are calculated by WinEpcas on the basis of  $\sum (A+M+T)=8.0$  normalization scheme. However, by selecting the *Apply Si=3 Normalization* option from the pull-down menu of *Si Normalization*, epidote formula is renormalized on  $Si=3.0$  (*apfu*), if the estimated Si (*apfu*) content of analysis exceeds 3.05. Using recalculated cations and anions of epidote-supergroup mineral analyses, the program first assigns four epidote subgroups including clinozoisite, allanite, dollaseite, and åskagenite and then determines the mineral species based on the dominant cations at *A1*, *A2*, *M1*, *M2*, *M3* as well as anions at *O4* and *O10* sites. All the calculated results by WinEpcas are stored in an output Excel file and, thus it can be used by users for further general data manipulation and graphing purposes. WinEpcas is distributed as a self-extracting setup file, including the necessary support files used by program, a help file, and sample data files.

Keywords: Epidote-supergroup; clinozoisite; allanite; dollaseite; åskagenite; classification; software.

### INTRODUCTION

Epidote-supergroup minerals, with complex solid solutions series, occur in a wide variety of paragenesis including magmatic and low to high metamorphic rocks, pegmatites, hydrothermal and metasomatic rocks, as well as in many ore deposit types. The minerals in this group are monoclinic in symmetry and have a topology consistent with space group  $P2_1/m$ . Epidote-supergroup minerals are members of the disilicate or sorosilicate structural family containing an isolated silicon tetrahedron and corner-sharing groups of two tetrahedra (Franz and Liebscher, 2004; Gieré and Sorensen, 2004). The structural formula of monoclinic epidote-supergroup minerals is represented as  $A_2M_3[T_2O_7][TO_4](O,F)(OH,O)$  or more clearly as

$A1A2M1M2M3(SiO_4)(Si_2O_7)O(OH)$  (Armbruster et al., 2006). In the structure of epidote-supergroup minerals, there exist two types of highly coordinated sites with the 9-coordinated *A1* and 10-coordinated *A2*, which are mainly occupied by Ca. In general, cations having large ionic radius (e.g. Sr, Pb, Ba, REE<sup>3+</sup>) enter into the *A2* site, but cations with ionic radius smaller than Ca (e.g. Mn<sup>2+</sup>) may substitute at the *A1* site. Trivalent cations including Al, Fe<sup>3+</sup>, Mn<sup>3+</sup>, Cr<sup>3+</sup> and V<sup>3+</sup>, on the other hand, locate at the octahedral *M1* and *M3* sites and Al completely fills the *M2* site, although a small amount of Ti<sup>4+</sup> also possibly substitutes at the *M2* site (Nagashima et al., 2011). However, in a coupled substitution between  $Ca^{2+}(A2)+M^{3+}(M3)$  and  $REE^{3+}(A2)+M^{2+}(M3)$ , divalent

cations such as Mg, Fe<sup>2+</sup> and Mn<sup>2+</sup> favor the *M3* site (Nagashima et al., 2010).

Although a variety of computer programs has been published for calculation and classification of rock-forming silicate minerals in recent years (e.g. Yavuz, 2001, 2003, 2007; Locock, 2008; Yavuz et al., 2014, 2015), software on classification of epidote-supergroup minerals, on the basis of the current IMA report (Armbruster et al., 2006), has not yet been appeared in literature. In this paper, we developed a computer program, called WinEpclas, using the Microsoft® Visual Basic programming language to calculate multiple mineral analyses obtained both from wet chemical and electron-microprobe techniques. WinEpclas estimates epidote-supergroup mineral analyses based on  $\sum$  cations=8.0 normalization scheme. However, the formula can be optionally renormalized on Si=3.0 if Si (*apfu*) content of epidote analysis is higher than 3.05. Classification of epidote-supergroup mineral names is carried out according to criteria proposed by the current IMA report (Armbruster et al., 2006), but with new mineral species approved by the Commission on New Minerals, Nomenclature and Classification [e.g. uedeite-(Ce), allanite-(Nd), ferriallanite-(La), vanadoallanite-(La), ferriakasaite-(La), ferriandrosite-(La), and åskagenite-(Nd)]. The program is capable to estimate the Fe<sup>3+</sup> and Fe<sup>2+</sup> contents from microprobe-derived total FeO (wt%) analysis and to calculate the Mn<sup>3+</sup> and Mn<sup>2+</sup> contents from given as Mn<sub>2</sub>O<sub>3</sub> (wt%) within the stoichiometric constraints. WinEpclas allows the user to display epidote-supergroup minerals in various binary and ternary classification and variation diagrams by using the Golden Software's Grapher program.

#### EPIDOTE-SUPERGROUP MINERALS NOMENCLATURE

Epidotes in monoclinic symmetry and a topology consistent with space group *P2<sub>1</sub>/m* were accepted by the subcommittee in defining epidote-supergroup minerals. Thus, zoisite, an orthorhombic polymorph of clinozoisite, is not considered as a member of epidote-supergroup minerals within this family. Epidote-supergroup minerals are described with the generic formula *A2M3*[*T2O7*][*TO4*](O,F)(OH,O). The monoclinic crystal structure includes *T2O7* and *TO4* units, where *T* corresponds usually to Si, linked to two kinds of chains. The first chain consists of the *M2* octahedra and the second chain is formed by the *M2* octahedra with the *M3* octahedra attached on alternate sides (Armbruster et al., 2006). In the generic formula of epidote-supergroup minerals, the *M* octahedra are generally occupied by trivalent cations including Al, Fe<sup>3+</sup>, Mn<sup>3+</sup>, Cr<sup>3+</sup> and V<sup>3+</sup>. Divalent cations such as Mg, Fe<sup>2+</sup> and Mn<sup>2+</sup> may occupy the *M* sites, preferentially the *M3* site, depending on various heterovalent substitutions. The *M2* site, to which usually an OH group is bounded

has a strong preference for Al, but occupancy of the *M1* and *M3* sites depends on competing cations. The overall structural arrangement in epidote-supergroup minerals causes two type of cavities hosting the *A1* and *A2* sites. The smaller *A1* is usually occupied by Ca or Mn<sup>2+</sup> and the larger *A2* is generally occupied by Ca, Sr, Pb and (REE)<sup>3+</sup> (Armbruster et al., 2006).

#### Definition of epidote-supergroup mineral subgroups

This group minerals are divided into three subgroups including clinozoisite, allanite and dollaseite (Armbruster et al., 2006). However, discovery of a new epidote-supergroup mineral åskagenite-(Nd) by Chukanov et al. (2010) changed the number of subgroups to four. Members of the clinozoisite subgroup are derived from the mineral clinozoisite Ca<sub>2</sub>Al<sub>3</sub>[Si<sub>2</sub>O<sub>7</sub>][SiO<sub>4</sub>]O(OH) only by homovalent substitutions. Minerals of the clinozoisite subgroup are named based on the key cations and anions at different structural sites [i.e. *A1*=M<sup>2+</sup>, *A2*=M<sup>2+</sup>, *M1*=M<sup>3+</sup>, *M2*=M<sup>3+</sup>, *M3*=M<sup>3+</sup>, *O4*=O<sup>2-</sup>, *O10*=(OH)]. Members of the allanite subgroup consist of (REE)<sup>3+</sup>-rich minerals typified by the eponymous mineral "allanite". The allanite subgroup is derived from clinozoisite by homovalent substitutions and one coupled heterovalent substitution of <sup>*A2*</sup>(REE)<sup>3+</sup>+<sup>*M3*</sup>M<sup>2+</sup>→<sup>*A2*</sup>Ca<sup>2+</sup>+<sup>*M3*</sup>M<sup>3+</sup> (Armbruster et al., 2006). Minerals of the allanite subgroup are named based on the valences of some elements at the key sites labelled with bold characters [i.e. *A1*=M<sup>2+</sup>, ***A2***=M<sup>3+</sup>, *M1*=M<sup>3+</sup>, *M2*=M<sup>3+</sup>, ***M3***=M<sup>2+</sup>, *O4*=O<sup>2-</sup>, *O10*=(OH)]. Dollaseite subgroup minerals also consist of REE<sup>3+</sup>-rich minerals typified by the eponymous mineral "dollaseite". This subgroup is derived from clinozoisite by homovalent substitutions and two coupled heterovalent substitutions of <sup>*A2*</sup>(REE)<sup>3+</sup>+<sup>*M3*</sup>M<sup>2+</sup>→<sup>*A2*</sup>Ca<sup>2+</sup>+<sup>*M3*</sup>M<sup>3+</sup> and <sup>*M1*</sup>M<sup>2+</sup>+<sup>*O4*</sup>F<sup>-</sup>→<sup>*M1*</sup>M<sup>3+</sup>+<sup>*O4*</sup>O<sup>2-</sup>. As in the allanite subgroup, minerals of the dollaseite subgroup are named based on the valences of some elements at the key sites labelled with bold characters [i.e. *A1*=M<sup>2+</sup>, ***A2***=M<sup>3+</sup>, ***M1***=M<sup>2+</sup>, *M2*=M<sup>3+</sup>, ***M3***=M<sup>2+</sup>, ***O4***=F<sup>-</sup>, *O10*=(OH)]. Åskagenite-(Nd), which is a new epidote-supergroup mineral described by Chukanov et al. (2010) is, at the same time, first representative of a new group with the *A1*<sup>2+</sup>*A2*<sup>3+</sup>*M1*<sup>3+</sup>*M2*<sup>3+</sup>*M3*<sup>3+</sup>(Si<sub>2</sub>O<sub>7</sub>)(SiO<sub>4</sub>)O<sub>2</sub> general formula. Åskagenite-(Nd), member of the åskagenite subgroup, is rich in (REE)<sup>3+</sup> and typified by the eponymous mineral "åskagenite". It seems that, minerals of the åskagenite subgroup may be named based on the valences of some elements at the key sites indicated by bold characters [i.e. *A1*=M<sup>2+</sup>, *A2*=M<sup>3+</sup>, *M1*=M<sup>3+</sup>, *M2*=M<sup>3+</sup>, ***M3***=M<sup>3+</sup>, ***O4***=O<sup>2-</sup>].

#### Derivation of epidote-supergroup minerals

In the clinozoisite subgroup, most frequent homovalent substitutions exist at the *M3* site by Fe<sup>3+</sup>, V<sup>3+</sup>, Cr<sup>3+</sup> and

$Mn^{3+}$ , as well at the  $A2$  site by  $Sr$ ,  $Pb^{2+}$  and less commonly  $Ba$ . These substitutions provide 20 combinations each corresponding to distinct mineral names (see rows 1-22 in Table 1). According to Armbruster et al. (2006), the key cation sites  $M3$  and  $A1$  control the root name. In other words, if the dominant cations at  $A1$  and  $M3$  sites fully match those of an approved species, then the same root name should be given to the discovered epidote-super group mineral. However, if at one of these sites the dominant cation is different then a new root name may be proposed. In clinozoisite and allanite (see rows 23-42 in Table 1) subgroups, no prefix is added to the root name if  $Al$  fully occupies the  $M1$  site. Similarly, in the dollaseite (see rows 43-46 in Table 1) subgroup, no prefix is added to the root name if  $Mg$  fully occupies the  $M1$  site. The prefixes ferri, mangani, chromo, and vanado in Table 1 for clinozoisite and allanite subgroups represent the dominant  $Fe^{3+}$ ,  $Mn^{3+}$ ,  $Cr^{3+}$ ,  $V^{3+}$  at the  $M1$  site, respectively. The prefixes ferro and mangano in the dollaseite subgroup (see Table 1) show dominant  $Fe^{2+}$  and  $Mn^{2+}$  at the  $M1$  site, respectively. On the other hand, the dominant cations such as  $Sr$  and  $Pb$ , substituting  $Ca$ , at the  $A2$  site for the clinozoisite group are defined as an *extended Levinson suffix* (see references in Armbruster et al., 2006). In the allanite, dollaseite and åskagenite subgroups, the  $A2$  site is dominantly occupied by rare earth elements and thus for these epidote-super group minerals Levinson suffixes *per se* are applied to the dominant rare earth element (REE) contents. Taking into account this simple nomenclature, Armbruster et al. (2006) proposed to rename some of previously used epidote minerals such as *niigataite*, *hancockite*, *strontio Piemontite*, *tweddillite* and *androsite* to clinozoisite-( $Sr$ ), epidote-( $Pb$ ), piemontite-( $Sr$ ), manganipiemontite-( $Sr$ ) and manganipiemontite-( $La$ ), respectively (see Table 1). However, Revheim and King (2016) suggested to instate the names *hancockite*, *niigataite* and *tweddillite* instead of epidote-( $Pb$ ), clinozoisite-( $Sr$ ) and manganipiemontite-( $Sr$ ) by referencing the recent IMA guidelines (Hatert et al., 2013) on priority to the historical provenance of names over nomenclature consistency.

#### Assigning subgroups and epidote-super group mineral names

In naming the epidote-super group minerals, priority is given to the preference of subgroup, then root name, and finally the specific name. In order to assign subgroups properly, we have to determine the dominant valence states at the  $M3$ ,  $M1$  and  $A2$  sites defined as  $M^{2+}$  and  $M^{3+}$ . Furthermore, the dominant valence at  $O4$  (e.g.  $O^{2-}$ ,  $F^-$ ) should be taken into account. Armbruster et al. (2006) suggested that clinozoisite, allanite and dollaseite subgroups can be classified on the basis of following scheme:

- i) If  $[M^{2+}]_{A2} > 0.50$  and  $[M^{3+}]_{M3} > 0.50$  then clinozoisite group,
- ii) If  $[M^{3+} + M^{4+}]_{A2} > 0.50$  and  $[M^{2+}]_{M3} > 0.50$  then allanite subgroup,
- iii) If  $\{[M^{2+}]_{M3+M1} - [M^{3+} + M^{4+}]_{A2}\} > 0.50$  and  $[X^-]_{O4} > 0.50$  then dollaseite subgroup.

Åskagenite-(Nd), which belongs to the åskagenite subgroup, is classified in the allanite subgroup according to the current epidote group nomenclature by Armbruster et al. (2006). However, this subgroup may be distinguished from the allanite subgroup based on the following scheme:

- iv) If  $[M^{2+}]_{M3} < 0.50$  and  $[M^{3+}]_{M3} > 0.50$  and  $[M^{3+}]_{M1} > 0.95$  and  $[M^{2+}]_{A2} = 0$  then åskagenite subgroup.

Epidote-super group mineral names of the clinozoisite subgroup are assigned on the basis of dominant cations at key structural sites for only homovalent substitutions. Although the root name depends on the dominant trivalent cations at the  $M3$  site, divalent cations such as  $Ca$ ,  $Sr$  and  $Pb$  at the  $A2$  site are considered in naming the clinozoisite subgroup minerals, in spite of the REE-bearing species. Armbruster et al. (2006) pointed out that for the sites a heterovalent substitution at the  $A2$  site (i.e. the  $M3$  site in the allanite subgroup and the  $M1$  site in the dollaseite subgroup), the relevant end-member formula must consider the dominant charge-compensating octahedral cation (e.g.  $M^{2+}$ ), but not the dominant cation at these sites.

#### Normalization and procedure for ionic species at key sites

Armbruster et al. (2006) recommended normalization of electron-microprobe-derived epidote-super group mineral analyses on the basis of  $\sum (A+M+T)=8.0$  procedure. However, this approach is inadequate both for vacancies at the  $A$  site and all elements that are not analyzed by electron-microprobe technique. In either case, this method leads to  $Si > 3.0$  apfu and in case of  $Si > 3.05$  apfu, the epidote formula may be renormalized on  $Si=3.0$ . However, according to Ercit (2002), renormalization to  $Si=3.0$  transfers all errors in  $Si$  determination to other cations in the formula. The cations of epidote-super group mineral analyses are allocated to the  $T$ ,  $M$  and  $A$  sites by program as follows:

- i) All  $Si$  (apfu) is assigned to the  $T$  site. If  $Si < 3.0$ , then  $Al^{IV}$  (apfu) is calculated as  $3.0 - Si$ ,
- ii) If there is sufficient  $Al$  after step i), then the  $M2$  site is fully occupied by  $Al$ ,
- iii) Any excess (oct-2.0) of octahedral cations (oct =  $Al$ ,  $Cr^{3+}$ ,  $V^{3+}$ ,  $Fe^{3+}$ ,  $Mn^{3+}$ ,  $Ti^{4+}$ ,  $Sn^{4+}$ ,  $Nb^{5+}$ ,  $Fe^{2+}$ ,  $Mn^{2+}$ ,  $Mg$ ,  $Cu^{2+}$ ,  $Ni^{2+}$ ,  $Zn^{2+}$ ) is to be assigned to the  $A1$  site. Priority is given to  $Mn^{2+}$ . If the amount of  $Mn^{2+}$  is not sufficient, then preference is given to  $Fe^{2+}$  or other available cations with large ionic radii as outlined by Armbruster et al. (2006).

Table 1. Classification of epidote-supergruop minerals based on the dominant cations and anions at key sites (revised from Armbruster et al., 2006).

Row	Name	A1	A2	M1	M2	M3	O4	O10
Clinozoisite subgroup								
1	<b>Clinozoisite</b>	Ca	Ca	Al	Al	Al	O	OH
2	<b>Clinozoisite-(Sr)<sup>*a</sup></b>	Ca	Sr	Al	Al	Al	O	OH
3	Clinozoisite-(Pb) <sup>§</sup>	Ca	Pb	Al	Al	Al	O	OH
4	<b>Epidote</b>	Ca	Ca	Al	Al	Fe <sup>3+</sup>	O	OH
5	<b>Epidote-(Pb)<sup>*b</sup></b>	Ca	Pb	Al	Al	Fe <sup>3+</sup>	O	OH
6	Epidote-(Sr) <sup>§</sup>	Ca	Sr	Al	Al	Fe <sup>3+</sup>	O	OH
7	Ferriepidote <sup>§</sup>	Ca	Ca	Fe <sup>3+</sup>	Al	Fe <sup>3+</sup>	O	OH
8	Ferriepidote-(Sr) <sup>§</sup>	Ca	Sr	Fe <sup>3+</sup>	Al	Fe <sup>3+</sup>	O	OH
9	Ferriepidote-(Pb) <sup>§</sup>	Ca	Pb	Fe <sup>3+</sup>	Al	Fe <sup>3+</sup>	O	OH
10	Vanadoepidote <sup>§</sup>	Ca	Ca	V <sup>3+</sup>	Al	Fe <sup>3+</sup>	O	OH
11	Vanadoepidote-(Sr) <sup>§</sup>	Ca	Sr	V <sup>3+</sup>	Al	Fe <sup>3+</sup>	O	OH
12	Vanadoepidote-(Pb) <sup>§</sup>	Ca	Pb	V <sup>3+</sup>	Al	Fe <sup>3+</sup>	O	OH
13	<b>Mukhinite</b>	Ca	Ca	Al	Al	V <sup>3+</sup>	O	OH
14	Mukhinite-(Sr) <sup>§</sup>	Ca	Sr	Al	Al	V <sup>3+</sup>	O	OH
15	Mukhinite-(Pb) <sup>§</sup>	Ca	Pb	Al	Al	V <sup>3+</sup>	O	OH
16	Cr <sup>3+</sup> -rich clinozoisite <sup>§</sup>	Ca	Ca	Al	Al	Cr <sup>3+</sup>	O	OH
17	Chromotawmawite <sup>§</sup>	Ca	Ca	Cr <sup>3+</sup>	Al	Cr <sup>3+</sup>	O	OH
18	<b>Piemontite</b>	Ca	Ca	Al	Al	Mn <sup>3+</sup>	O	OH
19	<b>Piemontite-(Sr)<sup>*c</sup></b>	Ca	Sr	Al	Al	Mn <sup>3+</sup>	O	OH
20	Piemontite-(Pb) <sup>§</sup>	Ca	Pb	Al	Al	Mn <sup>3+</sup>	O	OH
21	Manganipiemontite <sup>§</sup>	Ca	Ca	Mn <sup>3+</sup>	Al	Mn <sup>3+</sup>	O	OH
22	<b>Manganipiemontite-(Sr)<sup>*d</sup></b>	Ca	Sr	Mn <sup>3+</sup>	Al	Mn <sup>3+</sup>	O	OH
Allanite subgroup								
23	<b>Allanite-(Ce), -(La), -(Y)</b>	Ca	(REE) <sup>3+</sup>	Al	Al	Fe <sup>2+</sup>	O	OH
24	<b>Allanite-(Nd)<sup>†</sup></b>	Ca	Nd <sup>3+</sup>	Al	Al	Fe <sup>2+</sup>	O	OH
25	<b>Ferriallanite-(Ce)</b>	Ca	Ce <sup>3+</sup>	Fe <sup>3+</sup>	Fe <sup>3+</sup>	Fe <sup>2+</sup>	O	OH
26	<b>Ferriallanite-(La)<sup>†</sup></b>	Ca	La <sup>3+</sup>	Fe <sup>3+</sup>	Fe <sup>3+</sup>	Fe <sup>2+</sup>	O	OH
27	Vanadoallanite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	V <sup>3+</sup>	Al	Fe <sup>2+</sup>	O	OH
28	<b>Vanadoallanite-(La)<sup>†</sup></b>	Ca	La <sup>3+</sup>	V <sup>3+</sup>	Al	Fe <sup>2+</sup>	O	OH
29	Chromoallanite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	Cr <sup>3+</sup>	Al	Fe <sup>2+</sup>	O	OH
30	<b>Dissakisite-(Ce), -(La)</b>	Ca	(REE) <sup>3+</sup>	Al	Al	Mg	O	OH
31	Ferridissakisite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	Fe <sup>3+</sup>	Al	Mg	O	OH
32	Vanadodissakisite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	V <sup>3+</sup>	Al	Mg	O	OH
33	Manganidissakisite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	Mn <sup>3+</sup>	Al	Mg	O	OH
34	Chromodissakisite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	Cr <sup>3+</sup>	Al	Mg	O	OH
35	Androsite-(REE) <sup>§</sup>	Mn <sup>2+</sup>	(REE) <sup>3+</sup>	Al	Al	Mn <sup>2+</sup>	O	OH
36	<b>Manganianandrosite-(La)<sup>*</sup>, -(Ce)<sup>e</sup></b>	Mn <sup>2+</sup>	(REE) <sup>3+</sup>	Mn <sup>3+</sup>	Al	Mn <sup>2+</sup>	O	OH

Table 1. ... Continued

Row	Name	A1	A2	M1	M2	M3	O4	O10
37	Ferriandrosite-(REE) <sup>§</sup>	Mn <sup>2+</sup>	(REE) <sup>3+</sup>	Fe <sup>3+</sup>	Al	Mn <sup>2+</sup>	O	OH
38	<b>Ferriandrosite-(La)<sup>†</sup></b>	Mn <sup>2+</sup>	La <sup>3+</sup>	Fe <sup>3+</sup>	Al	Mn <sup>2+</sup>	O	OH
39	<b>Vanadoandrosite-(Ce)</b>	Mn <sup>2+</sup>	Ce <sup>3+</sup>	V <sup>3+</sup>	Al	Mn <sup>2+</sup>	O	OH
40	Chromoandrosite-(REE) <sup>§</sup>	Mn <sup>2+</sup>	(REE) <sup>3+</sup>	Cr <sup>3+</sup>	Al	Mn <sup>2+</sup>	O	OH
41	<b>Uedaite-(Ce)<sup>†</sup></b>	Mn <sup>2+</sup>	Ce <sup>3+</sup>	Al	Al	Fe <sup>2+</sup>	O	OH
42	<b>Ferriakasaite-(La)<sup>†</sup></b>	Ca	La <sup>3+</sup>	Fe <sup>3+</sup>	Al	Mn <sup>2+</sup>	O	OH
Dollaseite subgroup								
43	<b>Dollaseite-(Ce)</b>	Ca	Ce <sup>3+</sup>	Mg	Al	Mg	F	OH
44	<b>Khristovite-(Ce)</b>	Ca	Ce <sup>3+</sup>	Mg	Al	Mn <sup>2+</sup>	F	OH
45	Ferrokhrystovite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	Fe <sup>2+</sup>	Al	Mn <sup>2+</sup>	F	OH
46	Manganokhrystovite-(REE) <sup>§</sup>	Ca	(REE) <sup>3+</sup>	Mn <sup>2+</sup>	Al	Mn <sup>2+</sup>	F	OH
Åskagenite subgroup								
47	<b>Åskagenite-(Nd)<sup>†</sup></b>	Mn <sup>2+</sup>	(REE) <sup>3+</sup>	Al	Al	Fe <sup>3+</sup>	O	O

Notes: Minerals in bold format show the IMA-approved epidote-supergrout species which are listed in the subcommittee report (Armbruster et al., 2006); (\*) = recommended new mineral names for accepted species in the subcommittee report (Armbruster et al., 2006) that correspond to old (a) = *Niigataite*, (b) = *Hancockite*, (c) = *Strontio Piemontite*, (d) = *Tweddillite* and (e) = *Androsite*, respectively; (§) = suggested by Armbruster et al. (2006) for epidote-supergrout minerals that require the IMA approval if they are newly described; (†) = new epidote-supergrout minerals approved by the IMA later than the subcommittee report by Armbruster et al. (2006).

iv) The A1 site is filled with Ca (*apfu*) to sum up to 1.0. Minor amount of Na (*apfu*) will also be assigned to the A1 site,

v) All (REE)<sup>3+</sup> together with Th<sup>4+</sup> and U<sup>4+</sup> (*apfu*) are assigned to the A2 site. Larger divalent cations such as Sr<sup>2+</sup>, Pb<sup>2+</sup>, Ba<sup>2+</sup> and K<sup>+</sup> (*apfu*) are also added to the A2 site. Remaining Ca (*apfu*) from the A1 site is added to the A2 site,

vi) If any, F and Cl (*apfu*) is assigned to the O4 site,

vii) The remaining 2.0 octahedral cations are assigned to the M3 and M1 sites.

## DESCRIPTION OF PROGRAM

WinEpclas is a compiled program developed for the Microsoft® Windows platform users. The program is written to calculate and classify epidote-supergrout minerals based on the IMA subcommittee report (Armbruster et al., 2006) with discovered and IMA-approved new epidote minerals since then. Calculations and classifications of all epidote-supergrout mineral analyses by WinEpclas are carried out in two windows called the *Data Entry Screen* and *Calculation Screen*, respectively. A list of the calculation steps in the *Calculation Screen* of program is given in Table 2. WinEpclas presents 12 binary and ternary classification and variation plots for epidote-

supergrout mineral analyses. These plots are displayed by the Golden Software's Grapher program by selecting diagram types from the pull-down menu of *Graph* in the *Calculation Screen* of WinEpclas.

Calculation of mineral compositions is carried out on the basis of 12.5 oxygens and total cations equal to 8.0. However, by selecting the *Apply Si=3 Normalization* option from the pull-down menu of *Si Normalization* in the *Data Entry Screen*, the program renormalizes calculated cations on the basis Si=3.0. For the epidote-supergrout mineral analyses in which iron content is given solely as FeO (i.e. for electron-microprobe analysis), stoichiometric constraints are considered to calculate the Fe<sup>2+</sup>/Fe<sup>3+</sup> following the Droop's (1987) method (e.g. see S1, S2, S10 and S11 in Table 3). Similarly, stoichiometric constraints are taken into account to calculate the Mn<sup>2+</sup>/Mn<sup>3+</sup> (e.g. see S6 and S8 in Table 3) by WinEpclas when manganese content is given solely as Mn<sub>2</sub>O<sub>3</sub> (wt%).

"We used the Inno Setup Compiler (Version 5.6.1; Russell and Laan, 2018) to create a self-extracting setup file (12.1 Mb)". WinEpclas runs as a single executable file on a computer where the Microsoft® Visual Studio (MVP) package is installed. However, with the help of necessary ".ocx" and ".dll" support files in the self-extracting setup file, the users can execute the program



Table 2. Description of column numbers in the *Calculation Screen* window of WinEpclas program and an output Excel file.

Row	Explanations	Column Numbers
1	Major oxide epidote–supergroup mineral analyses (wt%)	1-45
2	Blank	46
3	Recalculated cations of epidote–supergroup mineral analyses ( <i>apfu</i> )	47-89
4	Blank	90
5	Cations allocation at the <i>T</i> site	91-93
6	Cations allocation at the <i>M</i> site	94-108
7	Cations allocation at the <i>A</i> site	109-121
8	Blank	122
9	Dominant cations at the key sites	123-128
10	Classification of epidote–supergroup mineral subgroups	129
11	Classification of epidote–supergroup mineral names	130

Note : *apfu* = Atoms per formula unit.

without requiring the MVP package. WinEpclas runs properly in a personal computer with the 32-bit operating system. The MSFLXGRD.OCX file is necessary to execute WinEpclas program. If this file is not installed in the Windows operating system or version is older than in the operating system, then a windows appears on screen showing “Component ‘msflexgrd.ocx’ or one of its dependencies not correctly registered: a file is missing or invalid” just after an installation of program. In this case, users can execute WinEpclas program in personal computers with the Windows 7 or later operating system by applying procedures listed in Appendix. Following an installation of program setup file on the computer, the start-up screen with various pull-down menus and shortcuts appears on the screen. Execution of program may also be started by clicking the WinEpclas icon from All Programs options or program icon came-up with the installation on the desktop.

#### Data entry of epidote-supergroup mineral compositions

The users of WinEpclas can edit epidote-supergroup mineral analyses obtained from wet-chemical or electron-microprobe techniques by clicking the *New* icon on the tool bar, by selecting the *New File* from the pull-down menu of *File* option or pressing the *Ctrl + N* keys. The standard 43 variables are defined by program, including sample name and oxides (wt%) in the *Data Entry Screen* (Figure 1) for calculation and classification of mineral compositions in the following order:

Sample No, SiO<sub>2</sub>, TiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, V<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>,

Mn<sub>2</sub>O<sub>3</sub>, FeO, MgO, MnO, NiO, CuO, PbO, ZnO, BaO, CaO, SrO, Na<sub>2</sub>O, K<sub>2</sub>O, P<sub>2</sub>O<sub>5</sub>, Nb<sub>2</sub>O<sub>5</sub>, SnO<sub>2</sub>, La<sub>2</sub>O<sub>3</sub>, Ce<sub>2</sub>O<sub>3</sub>, Pr<sub>2</sub>O<sub>3</sub>, Nd<sub>2</sub>O<sub>3</sub>, Sm<sub>2</sub>O<sub>3</sub>, Eu<sub>2</sub>O<sub>3</sub>, Gd<sub>2</sub>O<sub>3</sub>, Tb<sub>2</sub>O<sub>3</sub>, Dy<sub>2</sub>O<sub>3</sub>, Ho<sub>2</sub>O<sub>3</sub>, Er<sub>2</sub>O<sub>3</sub>, Tm<sub>2</sub>O<sub>3</sub>, Yb<sub>2</sub>O<sub>3</sub>, Lu<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, ThO<sub>2</sub>, UO<sub>2</sub>, F, Cl and H<sub>2</sub>O.

Epidote-supergroup mineral compositions typed in an Excel file with the extension of “.xls” and “.xlsx” as in the order, can be loaded into the program’s *Data Entry Screen* by clicking the *Open Excel File* option from the pull-down menu of *File*. By selecting the *Edit Excel File* option from the pull-down menu of *File*, epidote-supergroup mineral analyses can be typed in a blank Excel file (i.e. WinEpclas), stored in a different file name with the extension of “.xls” or “.xlsx”, and then loaded into the program’s *Data Entry Screen* by clicking the *Open Excel File* 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 WinEpclas.chm file on the screen.

#### Worked examples

The following examples show how WinEpclas can be used in calculation and classification for a variety of epidote-supergroup mineral compositions in different geological settings. Validity of WinEpclas outputs has been tested (see Table 3) with representative epidote-supergroup mineral analyses selected from literature (Peacor and Dunn, 1988; Pautov et al., 1993; Nagasaki and Enami, 1998; Miyajima et al., 2003; Cenki-Tok et al., 2006; Armbruster et al., 2006; Miyawaki et al., 2008;

Table 3. Chemical compositions of epidote-supergroup minerals with calculations and classifications by WinEplac program.

Row	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12
SiO <sub>2</sub>	34.38	33.62	37.60	35.49	34.76	31.81	28.90	32.24	30.91	33.52	32.14	31.06
TiO <sub>2</sub>	0.49	0.31	0.06	0.75	0.00	0.03	0.00	0.00	0.00	0.44	0.21	0.00
Al <sub>2</sub> O <sub>3</sub>	13.93	16.88	28.40	24.86	19.35	14.34	14.04	11.85	17.48	18.16	15.61	15.42
Cr <sub>2</sub> O <sub>3</sub>	0.71	0.70	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.82	0.40	0.00
V <sub>2</sub> O <sub>3</sub>	8.89	8.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.78	8.46	0.00
Fe <sub>2</sub> O <sub>3</sub>	0.00	0.00	5.09	7.08	15.42	7.52	8.75	5.71	12.32	0.00	0.00	4.41
Mn <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	13.93	8.61	21.18	1.35	0.00	0.00	0.00
FeO	11.42	6.55	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.39	8.34	10.94
MgO	0.09	1.25	0.14	0.07	0.00	0.56	0.00	0.00	0.00	0.62	0.40	0.26
MnO	1.90	1.40	0.04	0.22	0.14	0.00	0.00	0.00	2.43	1.14	1.26	0.65
NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PbO	0.00	0.00	0.00	0.00	0.00	6.08	26.34	0.00	19.14	0.00	0.00	0.00
ZnO	0.00	0.00	0.00	0.00	0.00	0.74	0.00	0.00	0.00	0.00	0.00	0.00
BaO	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	17.78	14.24	22.00	14.09	15.91	12.08	11.86	10.03	11.54	14.82	11.76	9.92
SrO	0.00	0.00	2.66	14.75	10.76	0.00	0.00	18.53	3.55	0.00	0.00	0.00
Na <sub>2</sub> O	0.06	0.12	0.00	0.00	0.00	0.19	0.00	0.00	0.00	0.06	0.17	0.00
K <sub>2</sub> O	0.00	0.00	0.00	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00
P <sub>2</sub> O <sub>5</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
La <sub>2</sub> O <sub>3</sub>	3.88	6.74	0.00	0.00	0.00	3.88	0.00	0.00	0.00	7.48	4.23	0.22
Ce <sub>2</sub> O <sub>3</sub>	3.54	5.56	0.00	0.00	0.00	3.11	0.00	0.00	0.00	6.78	8.76	4.45
Pr <sub>2</sub> O <sub>3</sub>	0.20	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.38	1.43	1.62
Nd <sub>2</sub> O <sub>3</sub>	0.50	1.00	0.00	0.00	0.00	1.57	0.00	0.00	0.00	0.78	3.95	11.90
Sm <sub>2</sub> O <sub>3</sub>	0.10	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.21	0.57	4.59
Gd <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28	1.80
Tb <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.16
Dy <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.30	0.34
Er <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.13
Yb <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Y <sub>2</sub> O <sub>3</sub>	0.11	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.12	1.03
ThO <sub>2</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	0.00	0.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28	0.00	0.08
O=F	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12	0.00	0.03
H <sub>2</sub> O	0.00	0.00	0.00	1.77	0.00	0.00	1.47	1.45	1.54	0.00	0.00	1.51
Σ (wt%)	97.98	97.31	96.03	99.08	96.45	95.86	99.97	100.99	100.26	96.71	98.39	100.46
Si	2.977	2.990	2.998	3.001	3.002	3.012	2.950	2.927	2.963	3.023	2.972	3.003
Al <sup>IV</sup>	0.023	0.010	0.002	0.000	0.000	0.000	0.050	0.073	0.037	0.000	0.028	0.000
Σ T-site	3.000	3.000	3.000	3.001	3.002	3.012	3.000	3.000	3.000	3.023	3.000	3.003
Ti	0.032	0.021	0.004	0.048	0.000	0.002	0.000	0.000	0.000	0.030	0.015	0.000
Al <sup>VI</sup>	1.399	1.760	2.667	2.477	1.970	1.600	1.638	1.195	1.939	1.930	1.673	1.757
Cr	0.049	0.049	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.058	0.029	0.000
V	0.617	0.576	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.490	0.627	0.000
Fe <sup>3+</sup>	0.639	0.146	0.305	0.450	1.002	0.536	0.672	0.390	0.889	0.000	0.038	0.321

Table 3. ... Continued

Row	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12
Fe <sup>2+</sup>	0.188	0.282	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.331	0.562	0.885
Mg	0.012	0.166	0.017	0.009	0.000	0.079	0.000	0.000	0.000	0.083	0.055	0.037
Mn <sup>3+</sup>	0.000	0.000	0.000	0.000	0.000	0.576	0.669	1.390	0.099	0.000	0.000	0.000
Mn <sup>2+</sup>	0.065	0.000	0.003	0.016	0.010	0.155	0.000	0.024	0.074	0.077	0.000	0.000
Ni	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Zn	0.000	0.000	0.000	0.000	0.000	0.052	0.000	0.000	0.000	0.000	0.000	0.000
∑ M-site	3.000	3.000	2.998	3.000	2.982	3.000	2.979	3.000	3.000	3.000	3.000	3.000
Mn <sup>2+</sup>	0.074	0.105	0.000	0.000	0.000	0.273	0.000	0.049	0.123	0.010	0.099	0.053
Fe <sup>2+</sup>	0.000	0.059	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.045	0.000
Ca	1.650	1.357	1.879	1.276	1.472	1.226	1.297	0.976	1.185	1.432	1.165	1.028
Sr	0.000	0.000	0.123	0.723	0.539	0.000	0.000	0.976	0.197	0.000	0.000	0.000
Ba	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Pb	0.000	0.000	0.000	0.000	0.000	0.155	0.724	0.000	0.494	0.000	0.000	0.000
Na	0.010	0.021	0.000	0.000	0.000	0.035	0.000	0.000	0.000	0.010	0.030	0.000
K	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.000	0.000	0.000	0.000	0.000
P	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
REETotal	0.266	0.458	0.000	0.000	0.000	0.296	0.000	0.000	0.000	0.525	0.661	0.917
Th	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
∑ A-site	2.000	2.000	2.002	2.000	2.016	1.988	2.021	2.000	2.000	1.977	2.000	1.997
A1*	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca
A2*	Ca	Ca	Ca	Sr	Sr	Ca	Pb	Sr	Pb	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>
M1*	V	Al	Al	Al	Al	Al	Al	Mn <sup>3+</sup>	Al	Al	Al	Al
M2*	Al	Al	Al	Al	Al	Al	Al	Al	Al	Al	Al	Al
M3*	Fe <sup>3+</sup>	V	Al	Al	Fe <sup>3+</sup>	Mn <sup>3+</sup>	Mn <sup>3+</sup>	Mn <sup>3+</sup>	Fe <sup>3+</sup>	V	Fe <sup>2+</sup>	Fe <sup>2+</sup>
O4†	O	O	O	O	O	O	O	O	O	O	O	O
Subgroup	Czo	Czo	Czo	Czo	Czo	Czo	Czo	Czo	Czo	Aln	Aln	Aln
Name	Vanadoepidote	Mukhinite	Clinozoisite	Clinozoisite-(Sr)	Epidote-(Sr)	Piemontite	Piemontite-(Pb)	Manganipiemontite-(Sr)	Epidote-(Pb)	Allanite-(La)	Allanite-(Ce)	Allanite-(Nd)
Row	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24
SiO <sub>2</sub>	29.97	30.22	29.15	29.25	28.81	29.04	29.94	34.39	34.90	32.40	29.90	29.51
TiO <sub>2</sub>	1.01	2.24	0.75	0.86	0.06	1.26	0.00	0.00	0.00	0.00	1.60	0.00
Al <sub>2</sub> O <sub>3</sub>	7.64	10.37	9.35	9.61	9.65	8.20	16.02	18.55	18.89	8.90	9.50	15.85
Cr <sub>2</sub> O <sub>3</sub>	0.16	0.00	0.06	0.08	0.00	0.00	0.00	4.91	4.95	0.00	1.50	0.00
V <sub>2</sub> O <sub>3</sub>	7.64	0.00	4.11	3.40	5.30	0.00	0.00	0.00	0.00	0.00	1.10	0.00
Fe <sub>2</sub> O <sub>3</sub>	5.47	11.05	5.96	5.48	2.18	2.98	0.00	0.00	0.00	0.00	0.00	9.16
Mn <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	1.75	11.62	0.00	0.00	0.00	0.00	0.00	0.00
FeO	6.94	5.83	5.05	5.23	0.00	0.00	16.01	2.84	2.70	3.30	1.80	7.75
MgO	0.39	0.36	0.46	0.65	1.22	0.28	0.07	3.01	2.92	13.10	2.70	0.00
MnO	8.03	3.43	10.90	12.05	17.78	15.01	6.01	0.00	0.00	0.00	11.80	7.98
NiO	0.05	0.00	0.03	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PbO	0.00	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	0.00	0.00	0.00	0.00	0.00	0.00
BaO	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00



Table 3. ... Continued

Row	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24
CaO	6.97	9.46	5.38	4.26	2.57	3.82	2.42	13.95	14.19	9.20	5.60	0.27
SrO	0.16	0.00	0.01	0.04	0.00	1.17	0.00	0.00	0.00	0.00	0.00	0.00
Na <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K <sub>2</sub> O	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P <sub>2</sub> O <sub>5</sub>	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
La <sub>2</sub> O <sub>3</sub>	12.14	13.17	12.73	12.97	8.29	6.08	3.09	9.24	9.21	6.00	8.70	0.44
Ce <sub>2</sub> O <sub>3</sub>	3.75	11.58	5.25	5.25	16.14	12.22	10.75	9.43	9.08	13.20	13.60	7.99
Pr <sub>2</sub> O <sub>3</sub>	1.86	0.50	1.93	2.05	0.00	0.00	1.83	0.00	0.00	2.60	1.40	1.76
Nd <sub>2</sub> O <sub>3</sub>	4.94	0.57	4.97	5.16	0.84	3.24	6.44	1.29	1.31	6.00	4.20	11.21
Sm <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.18	1.35	0.24	0.24	2.40	0.60	3.01
Gd <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.48	0.00	0.00	0.54	0.00	0.00	2.10	0.00	0.00
Tb <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Dy <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.10	0.00
Er <sub>2</sub> O <sub>3</sub>	0.09	0.00	0.05	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Yb <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28
Y <sub>2</sub> O <sub>3</sub>	0.00	0.02	0.03	0.01	0.00	0.00	0.72	0.14	0.16	0.00	0.00	2.27
ThO <sub>2</sub>	0.00	3.64	0.00	0.00	0.00	0.00	0.51	0.00	0.00	0.00	0.00	0.72
F	0.07	0.00	0.05	0.28	0.57	0.07	0.00	0.00	0.00	3.00	2.00	0.00
O=F	0.03	0.00	0.02	0.12	0.24	0.03	0.00	0.00	0.00	1.26	0.84	0.00
H <sub>2</sub> O	2.75	0.00	3.17	3.01	1.44	1.45	1.50	0.00	0.00	2.02	1.50	0.55
∑ (wt%)	100.00	102.44	99.45	100.03	96.36	96.59	97.20	97.99	98.55	102.96	99.76	98.75
Si	3.027	2.977	3.001	3.010	3.019	3.034	3.025	3.000	3.000	2.990	3.000	2.994
Al <sup>IV</sup>	0.000	0.023	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010	0.000	0.006
∑ T-site	3.027	3.000	3.001	3.010	3.019	3.034	3.025	3.000	3.000	3.000	3.000	3.000
Ti	0.077	0.166	0.058	0.067	0.005	0.099	0.000	0.000	0.000	0.000	0.121	0.000
Al <sup>VI</sup>	0.909	1.181	1.135	1.165	1.192	1.010	1.908	1.907	1.914	0.958	1.123	1.890
Cr	0.013	0.000	0.005	0.007	0.000	0.000	0.000	0.339	0.336	0.000	0.119	0.000
V	0.619	0.000	0.339	0.280	0.445	0.000	0.000	0.000	0.000	0.000	0.088	0.000
Fe <sup>3+</sup>	0.325	0.819	0.462	0.424	0.172	0.234	0.103	0.207	0.194	0.233	0.143	0.699
Fe <sup>2+</sup>	0.586	0.480	0.435	0.450	0.000	0.000	0.979	0.000	0.000	0.000	0.008	0.411
Mg	0.059	0.053	0.071	0.100	0.191	0.044	0.011	0.391	0.374	1.802	0.404	0.000
Mn <sup>3+</sup>	0.000	0.000	0.000	0.000	0.140	0.924	0.000	0.000	0.000	0.000	0.000	0.000
Mn <sup>2+</sup>	0.408	0.286	0.493	0.505	0.856	0.689	0.000	0.000	0.000	0.000	0.993	0.000
Ni	0.004	0.000	0.002	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Zn	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
∑ M-site	3.000	2.985	3.000	3.000	3.000	3.000	3.000	2.844	2.818	2.993	3.000	3.000
Mn <sup>2+</sup>	0.279	0.000	0.457	0.545	0.722	0.639	0.514	0.000	0.000	0.000	0.009	0.686
Fe <sup>2+</sup>	0.000	0.000	0.000	0.000	0.000	0.000	0.271	0.000	0.000	0.000	0.000	0.247
Ca	0.754	0.998	0.594	0.470	0.289	0.428	0.262	1.304	1.307	0.910	0.602	0.029
Sr	0.009	0.000	0.001	0.002	0.000	0.071	0.000	0.000	0.000	0.000	0.000	0.000
Ba	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Pb	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Na	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 3. ... Continued

Row	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24
K	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
P	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
REE <sub>Total</sub>	0.840	0.935	0.940	0.974	0.971	0.829	0.916	0.652	0.632	1.076	1.144	1.021
Th	0.000	0.082	0.000	0.000	0.000	0.000	0.012	0.000	0.000	0.000	0.000	0.017
$\sum A$ -site	1.883	2.015	1.999	1.990	1.981	1.966	1.975	1.956	1.939	1.985	1.756	2.000
A1*	Ca	Ca	Ca	Mn <sup>2+</sup>	Mn <sup>2+</sup>	Mn <sup>2+</sup>	Mn <sup>2+</sup>	Ca	Ca	Ca	Ca	Mn <sup>2+</sup>
A2*	(REE) <sup>3+</sup>	REE+Th	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	REE+Th	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	(REE) <sup>3+</sup>	REE+Th
M1*	V	Fe <sup>3+</sup>	Fe <sup>3+</sup>	Fe <sup>3+</sup>	V	Mn <sup>3+</sup>	Al	Al	Al	Mg	Mg	Al
M2*	Al	Al	Al	Al	Al	Al	Al	Al	Al	Al	Al	Al
M3*	Fe <sup>2+</sup>	Fe <sup>2+</sup>	Mn <sup>2+</sup>	Mn <sup>2+</sup>	Mn <sup>2+</sup>	Mn <sup>2+</sup>	Fe <sup>2+</sup>	Mg	Mg	Mg	Mn <sup>2+</sup>	Fe <sup>3+</sup>
O4†	O	O	O	O	O	O	O	O	O	F	F	O
Subgroup	Aln	Aln	Aln	Aln	Aln	Aln	Aln	Aln	Aln	Dls	Dls	Akg
Name	Vanadoallanite-(REE)	Ferriallanite-(La)	Ferriakasaite-(La)	Ferriandrosite-(REE)	Vanadoandrosite-(Ce)	Manganianandrosite-(Ce)	Uedaite-(Ce)	Dissakisite-(Ce)	Dissakisite-(La)	Dollaseite-(Ce)	Khristovite-(Ce)	Åskagenite-(Nd)

Notes: The formulae were recalculated to 12.5 oxygens and total cations = 8.0; Fe<sup>3+</sup> and Fe<sup>2+</sup> estimations from total FeO (wt%) contents were carried out on the basis of stoichiometric constraints using Droop's (1987) method; (\*) = Dominant cation; (†) = Dominant anion; Czo = Clinzoisite; Aln = Allanite; Dls = Dollaseite; Akg = Åskagenite; S1, S2, S5, S6, S10, S11, S20 and S21 from Armbruster et al. (2006); S3 from Nagasaki and Enami (1998); S4 from Miyajima et al. (2003); S7 from Chukanov et al. (2012); S8 from ("Manganipiemontite-(Sr) analysis," 2018); S9 from ("Epidote-(Pb) analysis," 2018); S12 from Škoda et al. (2012); S13 from Nagashima et al. (2013); S14 from Kolitsch et al. (2012); S15, S16 from Nagashima et al. (2015); S17, S18 from Cenki-Tok et al. (2006); S19 from Miyawaki et al. (2008); S22 from Peacor and Dunn (1988); S23 from Pautov et al. (1993); S24 from Chukanov et al. (2010).

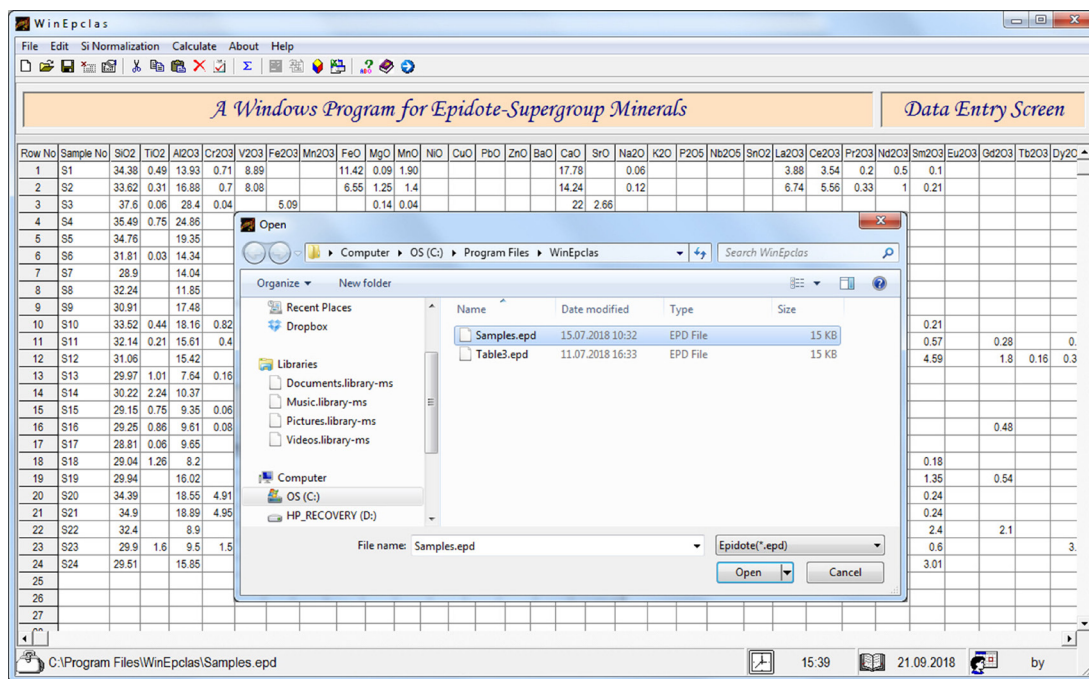


Figure 1. Screenshot of the WinEpclas *Data Entry Screen* window showing to open and edit previously typed epidote-supergroup mineral analyses.

Chukanov et al., 2010; Chukanov et al., 2012; Škoda et al., 2012; Kolitsch et al., 2012; Nagashima et al., 2013; Nagashima et al., 2015); ["Manganipiemontite-(Sr)

analysis," 2018], ["Epidote-(Pb) analysis," 2018].

Once the mineral analyses are processed by clicking the *Calculate* icon (i.e.  $\Sigma$ ) in the *Data Entry Section* of

the program, all estimation parameters are displayed in columns 1-130 (see Table 2) of the *Calculation Screen*. 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 “.epd”. By clicking the *Send results to Excel file* icon in the *Calculation Screen*, all calculations can be

stored in an Excel file (*Output.xlsx*) and then displayed by clicking the *Open and edit Excel file* icon. In an output Excel file, explanations can be displayed as comments provided that mouse cursor is on the second row of each column.

WinEpclas estimates cations of epidote-supergruop analyses (see rows 47-89 in Figure 2 a,b) and then

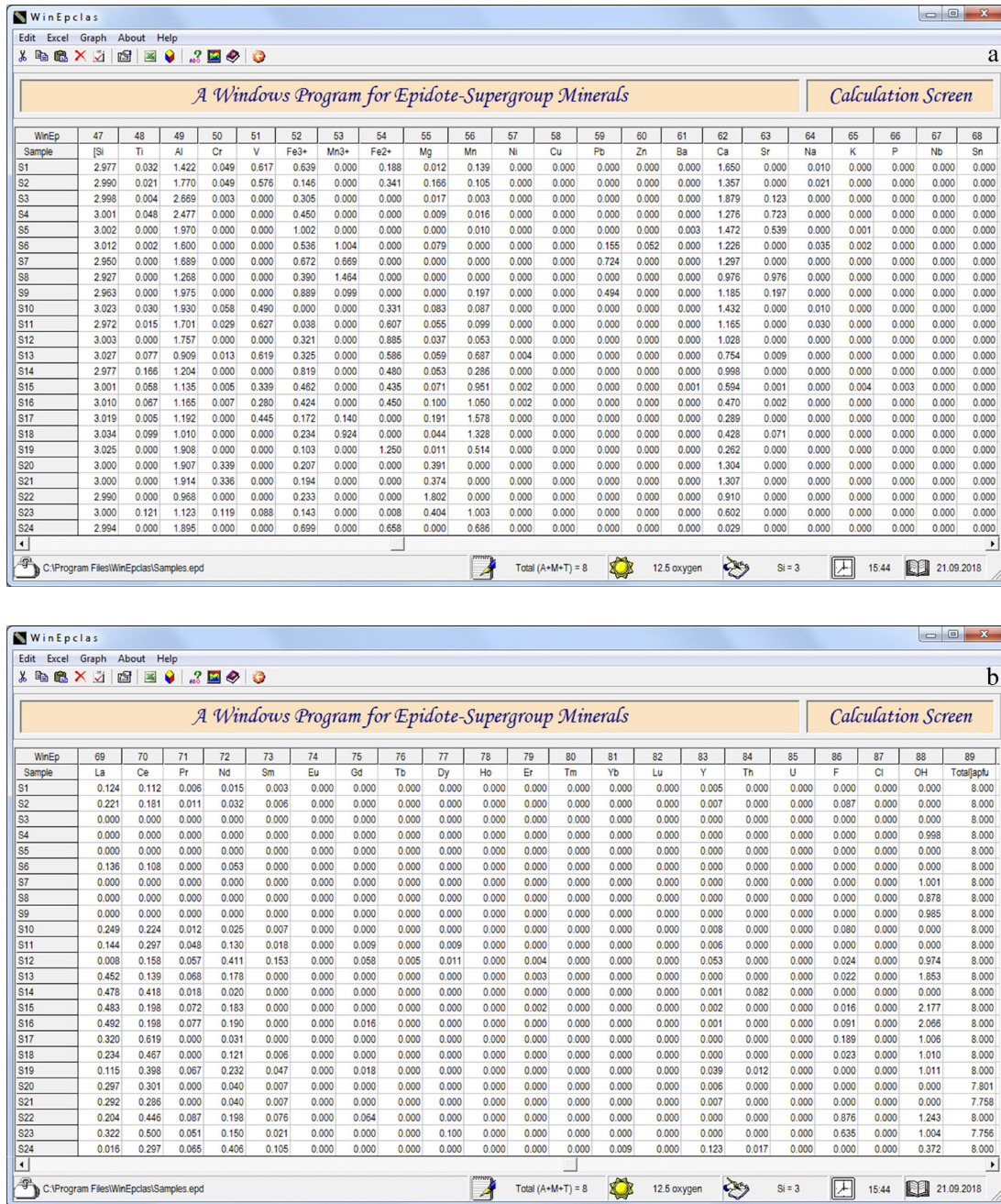


Figure 2. Screenshots of the WinEpclas *Calculation Screen* window showing (a, b) recalculated cations (*apfu*) of epidote-supergruop mineral analyses listed in Table 3, (c, d) allocation of recalculated cations (*apfu*) into the *T, M, A* sites with dominant cations at the key sites, epidote-supergruop subgruop names and corresponding mineral species.





based on the average chemical compositions. Chromium- and vanadium-bearing epidote-super group minerals were reported from a number of localities worldwide (e.g. Treloar, 1987; Nagashima et al., 2006; Bačik and Uher, 2010; Nagashima et al., 2013, 2018). However, those clinozoisite- and allanite subgroup minerals containing dominant trivalent cations such as  $\text{Cr}^{3+}$  and  $\text{V}^{3+}$  at the *M1* and *M3* sites are not common. For example, “tawmawite” which is analogue of the  $\text{Cr}^{3+}$ -rich clinozoisite is not yet a valid species until clear evidence showing that  $\text{Cr}^{3+}$  is the dominant cation at the *M3* site. Hence, WinEpclas names a epidote-super group mineral analysis with dominant cations Al and  $\text{Cr}^{3+}$  at the *M1* and *M3* sites, respectively as  $\text{Cr}^{3+}$ -rich clinozoisite instead of “tawmawite”. The users of WinEpclas should consider these situations in classification of the epidote-super group mineral analyses.

Franz and Liebscher (2004) proposed a ternary Al-Fe-Cr classification diagram for monoclinic epidote minerals including “tawmawite”, clinozoisite and epidote by applying the nomenclature of intermediate members of the 50% rule. They also pointed out that analogue diagrams for other solid solutions can be used in a similar manner. For this purpose, WinEpclas calculates the mol fraction of end members of clinozoisite subgroup such as “tawmawite” ( $X_{\text{Taw}}$ ), clinozoisite ( $X_{\text{Czo}}$ ), epidote ( $X_{\text{Ep}}$ ), mukhinite ( $X_{\text{Muk}}$ ) and piemontite ( $X_{\text{Pmt}}$ ) and displays them in three different ternary diagrams (see Figure 3 a,b,c) by clicking each graph type from the pull-down menu of *Clinozoisite Subgroup Plots* under the *Graph* in the *Calculation Screen* with the help of Grapher software. Epidote-super group minerals rich in rare earth elements (REE) comprise allanite, dollaseite and åskagenite subgroups. In these subgroups, allanite is common accessory phase in igneous, metamorphic, metasomatic and sedimentary rocks (Gieré and Sorensen, 2004). Small amounts of REE are present in most of epidote-super group minerals. However, in allanite, ferriallanite, dissakisite (i.e. Mg analogue of allanite), androsite, dollaseite, khristovite and åskagenite the REE are essential structural constituents allocated at the *A2* site. Similarly, classification of allanite species in ternary diagrams (see Figure 3 d,e,f) on the basis of dominant REE contents is displayed on screen by selecting the graph type from the pull-down menu of *Allanite Subgroup Plots* under the *Graph* option in the *Calculation Screen*.

#### SUMMARY AND AVAILABILITY OF THE PROGRAM

WinEpclas is developed for personal computers executing in the Windows operating system to calculate and classify monoclinic epidote-super group minerals crystallized in a variety of geological settings and rock types including magmatic, metamorphic, sedimentary and pegmatite, as well as hydrothermal and metasomatic

rocks. The program calculates multiple epidote-super group analyses on the basis of 12.5 oxygens and total cations equal to 8.0 obtained both from wet-chemical and electron-microprobe techniques. WinEpclas estimates the  $\text{Fe}^{2+}/\text{Fe}^{3+}$  and  $\text{Mn}^{2+}/\text{Mn}^{3+}$  from total FeO (wt%) and  $\text{Mn}_2\text{O}_3$  (wt%) contents within the stoichiometric constraints. The program generates two main windows. The first window (i.e. *Start-up/New File/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 new or load previously typed mineral analyses into the *Data Entry Screen* for a desired calculation scheme. By clicking the *Calculate* icon (i.e.  $\Sigma$ ) in the *Data Entry Screen*, all calculated parameters together with input mineral analyses are transferred to the second window (i.e. *Calculation Screen*).

The second window (i.e. *Calculation Screen*) allows the user to display these parameters on screen in a tabulated form between column numbers 1 and 130; including major oxide epidote-super group mineral compositions (wt%), recalculated cations (*apfu*) of analyses, allocation of those cations at the *T*, *M* and *A* sites, dominant cations at the key sites (e.g. *A1*, *A2*, *M1*, *M2*, *M3* and *O4*) and four type epidote-super group subgroup names with corresponding mineral species. All data in the *Calculation Screen* can be sent to a Microsoft® Excel file (i.e. output.xlsx) by clicking the *Send Results to Excel* icon or selecting same option from the pull-down *Excel* menu. Similarly, an output Excel file can be displayed by clicking the *Open Excel file* option from the pull-down menu of *Excel*. WinEpclas is a compiled program that consists of a self-extracting setup file, including support files for the Microsoft® Visual Studio package not installed on the computer, help file, data files (e.g. epd, xls, and xlsx), and Grapher plot document files (e.g. grf files). By clicking the setup file, the program and its associated files are installed into the directory of “C:\Program Files\WinEpclas” in the 32-bit operating system or “C:\Program Files (x86)\WinEpclas” in the 64-bit operating system. WinEpclas program requires the MSFLEXGRD.OCX registration in the Windows 7 or later personal computers with the 64-bit operating system (see Appendix). The self-extracting setup file is approximately 12.1 Mb and can be obtained from the journal server or corresponding author on request.

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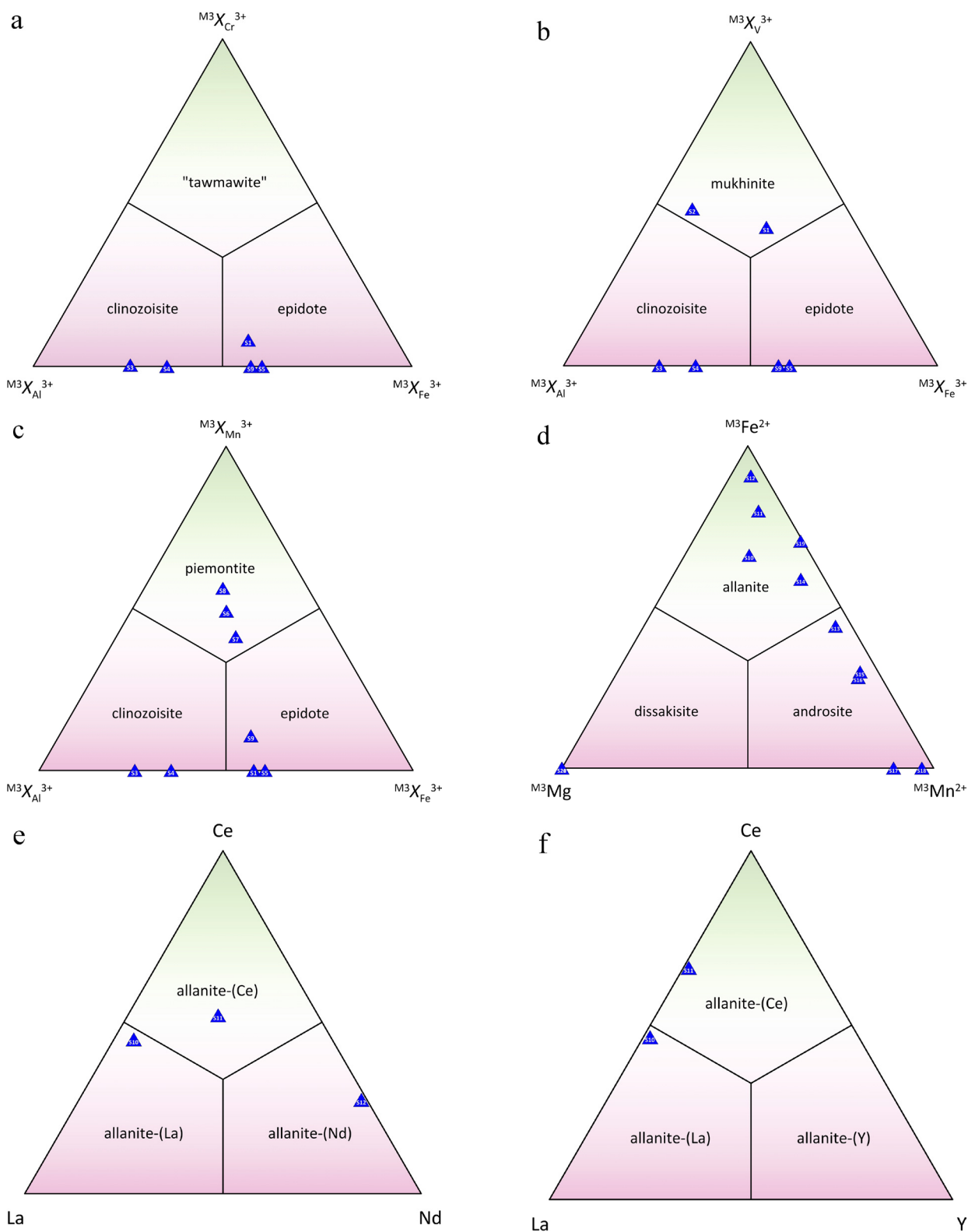


Figure 3. Nomenclature of monoclinic epidote-supergruop minerals belong to the clinozoisite subgroup in ternary (a)  $V^{3+}$ -Al- $Fe^{3+}$ , (b)  $V^{3+}$ -Al- $Fe^{3+}$  and (c)  $Mn^{3+}$ -Al- $Fe^{3+}$  diagrams (after Franz and Liebscher, 2004). (d) Ternary  $Fe^{2+}$ -Mg- $Mn^{2+}$  plot showing the composition of allanite subgroup minerals on the basis of dominant cations at the  $M3$  site (this study). (e, f) Ternary plots showing the composition of allanite minerals in terms of the three dominant lanthanide cations including Ce, La, Nd, as well as Y.



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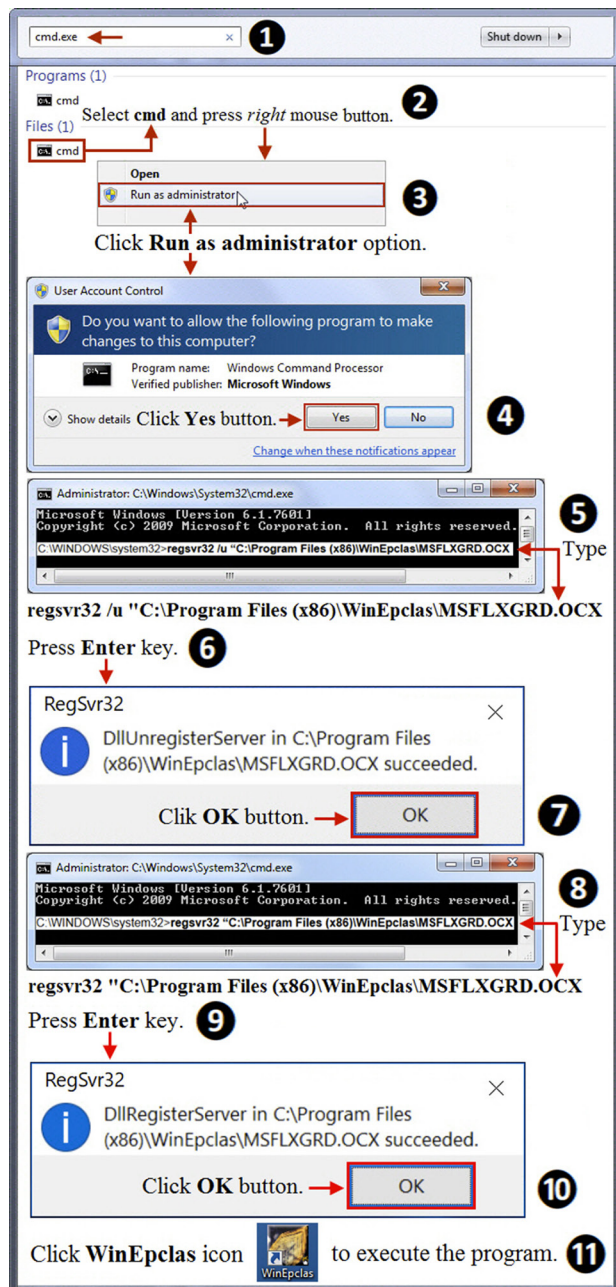
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## APPENDIX



Steps to execute the program in a personal computer with the 64-bit Windows 7 or later operating system.

1) Click **Start** button and type `cmd.exe` in the *Search programs and files* box.

2) Select `cmd` and press right mouse button.

3) Click **Run as administrator** option.

4) A windows appears on screen showing “Do you want to allow the following program to make changes to this computer?”. In this windows, click **Yes** button.

5) A black screen appears on screen starting with the `C:\Windows\system32>` command. In here, type `regsvr32 /u “C:\Program Files (x86)\WinEpclas\MSFLXGRD.OCX` and,

6) Press **ENTER** key.

7) You will see a windows on screen showing “DllUnregisterServer in C:\Program Files (x86)\WinEpclas\MSFLXGRD.OCX succeeded”. Press **OK** button to continue.

8) Type `regsvr32 “C:\Program Files (x86)\WinEpclas\MSFLXGRD.OCX` and,

9) Press **ENTER** key.

10) You will see a windows on screen showing “DllRegisterServer in C:\Program Files (x86)\WinEpclas\MSFLXGRD.OCX succeeded”. Press **OK** button to continue.

11) Finally, click **WinEpclas** icon on desktop to execute the program.

