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WinCrtclas, a Windows program for cerite-supergroup minerals†

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† *In memory of Ali Güzel, who made significant contributions to my academic career and passed away in 2024.*

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ABSTRACT

A Microsoft® Visual Basic software, WinCrtclas, has been developed to calculate the chemical formulas of cerite-supergroup minerals (CSM) based on data obtained from wet-chemical and electron-microprobe analyses. WinCrtclas currently evaluates 17 valid mineral species using the Commission on New Minerals, Nomenclature and Classification (CNMMC) of the International Mineralogical Association (IMA) nomenclature scheme in the general formula $A_9XM[T_7O_{24}Ø_4]Z_3$. The program recalculates the compositional formulas of CSM based on 28 oxygen atoms with the T-site total of 7.00 normalization option. Mineral formulas of the CSM are calculated considering the valency-imposed double site occupancy and the site total charge approach, allowing a double suffix to state the essential A constituents in the general formula. WinCrtclas operates in four stages: (1) it estimates cation and anion contents provided by input chemical data; (2) it determines the dominant cation and anion at the A, X, M, T and Z sites; (3) it assigns the CSM based on the dominant cations and anions at these sites; and (4) it classifies the species into an appropriate groups. WinCrtclas allows users to: (1) enter up to 41 input variables for mineral-chemical analyses; (2) type and load multiple CSM compositions in the data entry section; (3) edit and load the Microsoft® Excel files used in calculating, classifying, and naming the CSM, and (4) store all the calculated parameters in the output of a Microsoft® Excel file for further data evaluations.

Keywords: cerite supergroup; cerite subgroup; taipingite subgroup; merrillite subgroup; whitlockite subgroup; cerite-(CeCa); taipingite-(CeCa); merrillite; whitlockite; classification; software.

INTRODUCTION

The cerite-supergroup minerals, which are composed of two groups [i.e., cerite (silicates) and merrillite (phosphates)] of isostructural trigonal *R*3*c* (#161) minerals, involves three 8- and 9-fold coordinated *A* sites, one 6-fold coordinated *X* site, one octahedral *M* site, and three $[TO_3(Ø)]$ tetrahedral groups (Atencio and Azzi, 2020; Atencio et al., 2023). The general chemical formula of cerite-supergroup minerals can be expressed as $A_9XM[T_7O_{24}Ø_4]Z_3$, where the letters, except for O for oxygen, specify groups of atoms to be applied for the dominant ion (e.g., Ce, and Ca for A, and OH and F for Z) and valency rule as well as the endmember concept: A=**REE** (i.e., La-Lu and Y), **Ca**, **Sr**, Ba, K, **Na**, and □ (vacancy); X=□, **Ca**, **Na**, and $\mathbf{Fe^{2+}}$; M=**Mg**, $\mathbf{Fe^{2+}}$, $\mathbf{Fe^{3+}}$, **Al**, Cr, **Mn**, and Ni; T=**Si**, **P**, V^{5+}, Ti, U, and Th; Ø=O and OH; and Z=□, OH, and F, with the main cations at constituents such as A, X, M, and T being presented in bold (Atencio and Azzi, 2020; Atencio et al., 2023). The crystal structure of cerite-supergroup minerals consists of $[M(TO_4)_6]$ clusters that are interconnected by $[A_9X(TO_3Ø)]$ groups. In this context, the general

structural formula of cerite-supergroup minerals is $A1_3A2_3A3_3XM1[T1_3T2_3T3O_{24}Ø1_3Ø10]Z1Z2Z3$, where the letter Z represents the set of anions located at three nonequivalent $Z1$, $Z2$, and $Z3$ sites. According to Atencio et al. (2023), grouping atoms in this way over similar sites helps to prevent the proliferation of mineral species with end-member formulas based on the structural formula.

Although various computer programs applicable to the calculation and classification of rock-forming silicates, as well as ore-related minerals, have been developed over the past two decades (e.g., Yavuz, 1999, 2003, 2013; Yavuz et al., 2014, 2015; Yavuz and Yıldırım, 2018, 2020; Yavuz, 2021; Yavuz and Yavuz, 2022, 2023 a,b, 2024; Yavuz, 2024 a,b; Janoušek et al., 2024), those useful for the cerite-supergroup minerals, according to the current IMA report, have not yet appeared in the literature, possibly in part due to the lack of a recent classification system by Atencio and Azzi (2020). Taking this situation into consideration, a computer program called WinCrtclas has been developed using the Microsoft® Visual Basic programming language. It can be used to calculate the chemical formulas from up to 200 analyses obtained from both wet-chemical and electron-microprobe techniques. The program calculates the compositional formulas of cerite-supergroup minerals on the basis of 28 oxygen atoms (apfu). However, the program allows users to select the T-site total of 7.00 (apfu) normalization option from the pull-down menu of *Calculate Contents of Ions* in the *Start-up Screen* or *Data Entry Screen* for the compositional formulas of cerite group minerals. The calculation and classification procedures applied to cerite-supergroup minerals by WinCrtclas are carried out based on the currently accepted IMA nomenclature scheme by Atencio and Azzi (2020), with changes to the cerite group nomenclature by Atencio et al. (2023). Additionally, it takes into account new species (e.g., nipeiite-(Ce) and karwowskiite) that post-date the IMA report. WinCrtclas allows the user to display members of the cerite supergroup in several binary and ternary classification and compositional diagrams by using Golden Software's Grapher program.

CERITE-SUPERGROUP MINERALS NOMENCLATURE

Using the available data on the cerite supergroup species, Atencio and Azzi (2020) proposed a nomenclature and classification scheme for the members of the cerite-supergroup minerals, which has been approved by the IMA–CNMNC (see Table 1). The cerite-supergroup minerals nomenclature, consisting of the cerite and merrillite groups, is based on the dominant species of valence at each site. In the proposed new classification scheme of the cerite-supergraoup minerals (Atencio and Azzi, 2020), the authors proposed to use of "#" sign at the A, X and M sites to replace minor chemical elements that balance the charge. In this context, for example, merrillite and keplerite would have the formulas $(Ca,\#)_9(Na,\#)(Mg,\#)(PO_4)_7$ and $(Ca,\#)_9(Ca,\#)(Mg,\#)(PO_4)_7$, respectively (Galuskin et al., 2023). Due to the recent studies and discoveries of new members in the cerite and merrillite groups, in addition to those already described, the current nomenclature scheme approved by the Commission on New Minerals, Nomenclature and Classification (CNMMC) of the International Mineralogical Association (IMA) as well as the deficiency in endmember formulas with a double site occupation at the one site and mineral systematics based on the definition of the endmember formula (e..g, Bosi et al., 2019 a,b), has subsequently been subjected to some nomenclature and classification changes, mainly in the cerite-group, which is subdivided into two subgroups: cerite and taipingite (Atencio et al., 2023). The subdivision procedure for the cerite and taipingite subgroups was carried out based on the dominant OH and F anions at the Z site, respectively. In the current nomenclature rules, considering the valency-imposed double site occupancy method of Hatert and Burke (2008) and Hatert et al. (2013), as well as the site total charge approach of Bosi et al. (2019b), a double suffix was proposed by Atencio et al. (2023) to indicate the essential A constituents for the general chemical formula of the cerite-supergroup minerals. Taking into account these new rules, the following changes in mineral names of the cerite group have been deemed necessary: cerite-(Ce) to cerite-(CeCa), ferricerite-(La) to ferricerite-(LaCa), aluminocerite-(Ce) to aluminocerite-(CeCa), and taipingite-(Ce) to taipingite-(CeCa). In this context, aluminotaipingite-(CeCa), a new member of the cerite-supergroup minerals, has been defined by Campostrini et al. (2023) in the tapingite subgroup. In the cerite-supergroup minerals, the prefix ferri- [e.g., ferricerite-(LaCa)] or alumino- [e.g., aluminocerite-(CeCa)] is added to species if the M cations are dominated by Fe^{3+} or Al, respectively. In the case where the dominant M cation is Mg, no prefix will be used to define the member of the cerite-supergroup species. There are many synthetic compounds that are synthesized due to their important technological properties with the cerite structure available in the industrial sector, such as arsenates and vanadates (e.g., in the manufacturing of white light-emitting diodes, phosphors, and light converters), which may indicate the possibility of additional cerite-supergroup minerals species in the future (Atencio and Azzi, 2020; see references therein).

Phosphate, which is an important constituent of the merrillite group within the cerite-supergroup minerals, is also a vital chemical compound for life on Earth. It is used to store energy in adenosine triphosphate (ATP), in the structure of heredity in DNA and RNA, as well as in the phospholipid membranes that surround cells and

Table 1. A list of the IMA-approved species in the cerite supergroup (from Atencio and Azzi, 2020; Atencio et al., 2023).

Row	Species	Symbol	Formula	A_9	X	M	T7	O_{24}	$Ø_4$	Z_3	IMA status
	Cerite Group										
	Cerite Subgroup										
1	Cerite-(CeCa)	Crt-Ce	$(Ce_7Ca_2)Mg(SiO_4)_3(SiO_3OH)_4(OH)_3$	Ce_7Ca_2	□	Mg	Si	O	OH	OH	A
2	Ferricerite-(LaCa)	Fecrt-La	$(La_6Ca_3)Fe^{3+}(SiO_4)_3(SiO_3OH)_4(OH)_3$	La_6Ca_3	□	Fe^{3+}	Si	O	OH	OH	A
3	Aluminocerite-(CeCa)	Acrt-Ce	$(Ce_6Ca_3)Al(SiO_4)_3(SiO_3OH)_4(OH)_3$	Ce_6Ca_3	□	Al	Si	O	OH	OH	A
4	†Nipeiite-(Ce)	Npe-Ce	$Ce_9Fe^{3+}(SiO_4)_6[SiO_3(OH)](OH)_3$	Ce_9	□	Fe^{3+}	Si	O	O_3OH	OH	A
	Taipingite Subgroup										
5	Taipingite-(CeCa)	Tpg-Ce	$(Ce_7Ca_2)Mg(SiO_4)_3(SiO_3OH)_4F_3$	Ce_7Ca_2	□	Mg	Si	O	OH	F	A
6	Aluminotaipingite-(CeCa)	Atpg-CeCa	$(Ce_6Ca_3)Al(SiO_4)_3(SiO_3OH)_4F_3$	Ce_6Ca_3	□	Al	Si	O	OH	F	A
	Merrillite Group										
	Merrillite Subgroup										
7	Merrillite	Mer	$Ca_9NaMg(PO_4)_7$	Ca_9	Na	Mg	P	O	O	□	A
8	Ferromerrillite	Fmer	$Ca_9NaFe^{2+}(PO_4)_7$	Ca_9	Na	Fe^{2+}	P	O	O	□	A
9	Keplerite	Kep	$Ca_9(Ca_{0.5}□_{0.5})Mg(PO_4)_7$	Ca_9	$Ca_{0.5}□_{0.5}$	Mg	P	O	O	□	A
10	Matyhite	Myh	$Ca_9(Ca_{0.5}□_{0.5})Fe^{2+}(PO_4)_7$	Ca_9	$Ca_{0.5}□_{0.5}$	Fe^{2+}	P	O	O	□	A
11	Deynekoite	Dnk	$Ca_9Fe^{3+}(PO_4)_7$	Ca_9	□	Fe^{3+}	P	O	O	□	A
12	Changesite-(Y)	Cgs-Y	$(Ca_8Y)Fe^{2+}(PO_4)_7$	Ca_8Y	□	Fe^{2+}	P	O	O	□	A
13	†Karwowskiite	Krw	$Ca_9(Fe^{2+}_{0.5}□_{0.5})Mg(PO_4)_7$	Ca_9	$Fe^{2+}_{0.5}□_{0.5}$	Mg	P	O	O	□	A
	Whitlockite Subgroup										
14	Whitlockite	Wht	$Ca_9Mg(PO_4)_6(PO_3OH)$	Ca_9	□	Mg	P	O	O_3OH	□	A
15	Strontiowhitlockite	Swht	$Sr_9Mg(PO_4)_6(PO_3OH)$	Sr_9	□	Mg	P	O	O_3OH	□	A
16	Hedegaardite	Hed	$(Ca_8Na)(Ca_{0.5}□_{0.5})Mg(PO_4)_6(PO_3OH)$	Ca_8Na	$Ca_{0.5}□_{0.5}$	Mg	P	O	O_3OH	□	A
17	Wopmayite	Wop	$(Ca_6Na_3)Mn(PO_4)_3(PO_3OH)_4$	Ca_6Na_3	□	Mn	P	O	OH	□	A

A = Approved by the IMA; □ = Vacancy; (†) = nipeiite-(Ce) (Qu et al., 2024) and karwowskiite (Galuskin et al., 2024) are new cerite-supergroup species approved by the IMA, later than the subcommittee report by Atencio and Azzi (2020).

organelles. As it is suggested that phosphate is vital for the prebiotic formation of RNA on Earth and is the most common limiting nutrient on the planet, it can be used as an important indicator of past life on Earth. A decrease in phosphate serves as a biomarker in paleosols and is supported by phosphate minerals encapsulating microbial cells. Therefore, phosphates have previously been suggested as important targets for sample collection on Mars, and the study of phosphates is of critical importance in the astrobiological investigation of Mars (Hausrath et al., 2024 and references therein).

Meteorites preserve evidence of processes such as the formation of solar system, the origins of life on Earth, and the possibility of life in space. Hence, minerals within meteorites provide the unique samples in the search for answers about our solar system. In recent years, merrillite, the anhydrous endmember of the merrillite [$Ca_9NaMg(PO_4)_7$]-whitlockite [$Ca_9Mg(PO_4)_6(PO_3OH)$] solid solution series, has become an important species in studies (e.g., Hughes et al., 2006, 2008; Jolliff et al., 2006; Adcock et al., 2014, 2017a; McCubbin et al., 2014; Shearer et al., 2015; Xie et al., 2015; Jones et al., 2016; Słaby et al., 2017; Ward et al., 2017; Jia et al., 2020; Darling et al., 2021; Kaminsky and Zedgenizov, 2022; Hausrath et al., 2024) due to its relatively major reservoir for rare earth elements and being an anhydrous calcium phosphate mineral that is found commonly in different types of meteorites, as well as lunar and Martian rocks, which can be used to understand planetary magmatic compositions and conditions in terms of petrogenesis, thermodynamics, and surface processes (Jia et al., 2020). Although merrillite in Martian meteorites has been interpreted as evidence of water-limited late-stage Martian melts, recent studies on apatite that coexisted with merrillite in the same meteorites suggest a higher water content in the melts. For example, the variable composition and interrelated relationships of phosphate minerals found in Martian meteorites have been considered indicators of late-stage melting evolution. In this respect, the widespread presence of merrillite and its anhydrous structure have been interpreted as evidence that the late-stage melts on Mars were relatively dry (Adcock et al., 2017a). Although Kaminsky et al. (2022) reported the first find of merrillite [$Ca_3(PO_4)_2$] in a terrestrial environment as an inclusion in lower-mantle diamond, it is not a phenomenon that is frequently observed in terrestrial environments as a discrete mineral phase. However, it can be produced from a similar rare terrestrial mineral, whitlockite, typically associated with pegmatites, in laboratory conditions through a dehydrogenation process, such as heating it to 1000-1100 ºC. For example, Adcock et al. (2017 a,b) tested this hypothesis and showed that merrillite was produced from whitlockite during experimental shock events, with potential implications for interpreting these type of minerals for parent body volatile abundances.

PROGRAM DESCRIPTION

WinCrtclas is a user-friendly, compiled program package (≈14 Mb) developed for personal computers running on the Microsoft® Windows operating system. The program first calculates the cation and anion values (in apfu) from analyses made on cerite-supergroup by means of wet-chemical or electron-microprobe techniques and then uses these to classify the mineral into the IMA-approved species that belong to two groups, including cerite and merrillite, with four subgroups consisting of cerite, taipingite, merrillite, and whitlockite (see Table 1). A list of the calculation steps in the *Calculation Screen* and in the output of a Microsoft Excel file developed by the program is given in Table 2. Upon the successful installation of WinCrtclas, the start-up screen with various pull-down menus and equivalent shortcuts appears on the screen (Figure 1a). The program allows the user to input wet-chemical or electron-microprobe cerite-supergroup analytical data by clicking the *New* icon on the toolbar, by selecting the *New File* from the pull-down menu of the *File* option, or pressing the *Ctrl+N* keys (Figure 1b). Up to 41 chemical analytes (in wt%) are used by WinCrtclas in the following order:

Sample No, SiO_2, TiO_2, UO_2, ThO_2, Al_2O_3, Cr_2O_3, Fe_2O_3, Y_2O_3, La_2O_3, Ce_2O_3, Pr_2O_3, Nd_2O_3, Sm_2O_3, Eu_2O_3, Gd_2O_3, Tb_2O_3, Dy_2O_3, Ho_2O_3, Er_2O_3, Tm_2O_3, Yb_2O_3, Lu_2O_3, V_2O_5, P_2O_5, Nb_2O_5, Ta_2O_5, FeO, MnO, NiO, PbO, ZnO, MgO, SrO, CaO, BaO, Na_2O, K_2O, SO_3, F, Cl, and H_2O.

Data from the analysis of a cerite-supergroup mineral can also be input into a blank Excel file following the above order, saving it with the extension of ".xls" or ".xlsx". After this, it can be loaded into the *Data Entry Screen* of the program 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*, data can be inserted into a blank Excel file (i.e., MyCerite), saved using a different file name (with the extension of ".xls" or ".xlsx"), and then loaded into the *Data Entry Screen* of the program by clicking the *Open Excel File* option from the pull-down menu of *File*. Additional information about the data entry or similar topics can be accessed by pressing the F1 function key to display the WinCrtclas. chm file on the screen. The current version of WinCrtclas includes a total of 23 binary and ternary classification and compositional plots. Data on any of these plots can be displayed using the program Grapher by selecting the diagram type from the pull-down menu of *Graph* in the *Calculation Screen* of the program (Figure 1c).

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

Row	Explanations	Column Numbers
1	Major oxides from the cerite-supergroup mineral (CSM) compositions (wt%)	1-44
2	Blank	45
3	Estimation of the stoichiometric H_2O content (wt%)	46
4	Blank	47
5	Recalculated cations from the CSM compositions (apfu)	48-86
6	Blank	87
7	Recalculated F, Cl and OH contents from the CSM compositions (apfu)	88-91
8	Blank	92
9	Allocation of ions by program at the A-site (apfu)	93-100
10	Blank	101
11	Allocation of ions by program at the X-site (apfu)	102-108
12	Blank	109
13	Allocation of ions by program at the M-site (apfu)	110-119
14	Blank	120
15	Allocation of ions by program at the T-site (apfu)	121-129
16	Blank	130
17	Dominant ions at the sites (i.e., A, X, M, T, and Z)	131-135
18	Blank	136
19	Group name, subgroup name, and species from the CSM compositions	137-139
20	Blank	140

(apfu) = Atoms per formula unit.

WORKED EXAMPLES

Using the selected data set from literature as well as "Species.crt" file in the installation document (i.e., WinCrtclas setup file), examples are presented that show how WinCrtclas can be used in the determination of chemical formulas and cerite-supergroup minerals classification. The previously typed or loaded analyses are processed by clicking the *Calculate* icon (i.e., ∑) in the *Data Entry Screen* of the program, after which all input and estimation parameters are displayed in columns 1-139 (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 processing of a selected data file with the extension of ".crt" which refers to the cerite supergroup. 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.

The validity of program output has been tested with representative cerite group (see references in Table 3) and merrillite group (see references in Table 4) minerals selected from the literature. WinCrtclas calculates the compositional formula for a given cerite-supergroup mineral analysis on the basis of 28 oxygen atoms (apfu). Alternatively, by clicking the *Based on the T-site Total=7.00 (apfu) Normalization* option from the pull-down menu of *Calculate Contents of Ions* in the *Start-up Screen* or *Data Entry Screen*, the program calculates cerite-supergroup minerals according to the selected criteria that are suitable for the compositional formulae of cerite group minerals. All input and calculated parameters are presented in the *Calculation Screen* and Excel output file for the selected mineral analyses from the literature. Classification of a given analysis into its proper group and subgroup is carried out on the basis of the dominant cation and anion at sites such as A, X, M. T, and Z. WinCrtclas calculates the cerite-supergroup mineral analyses (e.g., see rows 1-79 in Table 3) and allocates the recalculated ions at the A (see rows 80-87 in Table 3), X (see rows 88-92 in Table 3), M (see rows 93-97 in Table 3), and T (see rows 98-102 in Table 3) sites. The determination of dominant constituents by the program at each site (see rows 103-107 in Table 3) with a group, subgroup, and specific species (see rows 108-110 in Table 3) based on the current cerite-supergroup nomenclature scheme is provided on the *Calculation Screen*, as well as in

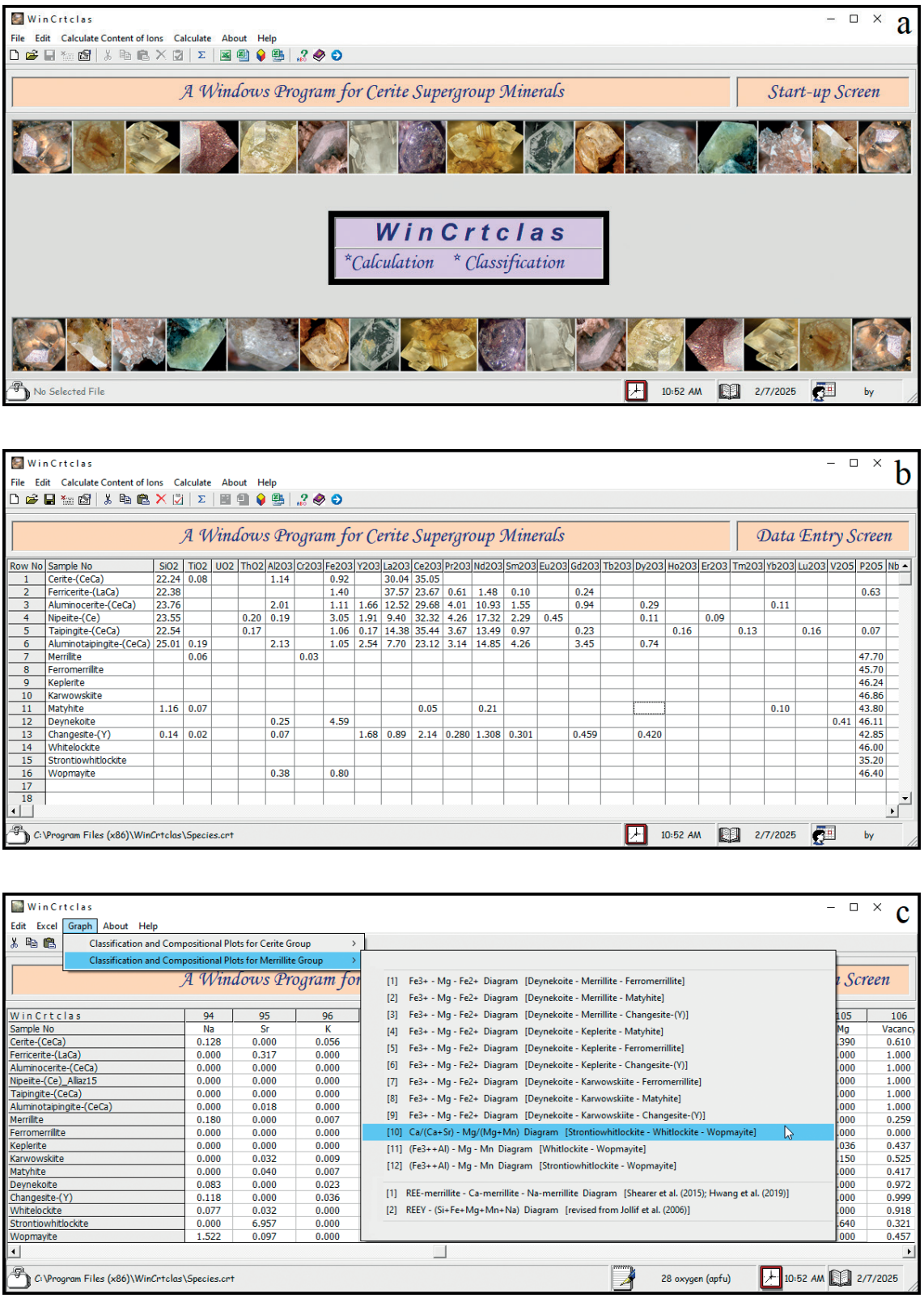

Figure 1. a) A screenshot of the WinCrtclas Start-up window with various pull-down menus and equivalent shortcuts. b) A screenshot of the WinCrtclas *Data Entry* window with a total of 41 analytes (wt%). c) A screenshot of the WinCrtclas *Calculation Screen* with plot options from the pull-down menu of the *Graph*.

Table 3. Chemical compositions of selected cerite group minerals with calculations and classifications by WinCrtclas.

Row		S1	S2	S3	S4	S5	S6
1	SiO_2	22.240	22.380	23.760	23.550	22.540	25.010
2	TiO_2	0.080	0.000	0.000	0.000	0.000	0.190
3	ThO_2	0.000	0.000	0.000	0.200	0.170	0.000
4	Al_2O_3	1.140	0.000	2.010	0.190	0.000	2.130
5	Fe_2O_3	0.920	1.400	1.110	3.050	1.060	1.050
6	Y_2O_3	0.000	0.000	1.660	1.910	0.170	2.540
7	La_2O_3	30.040	37.570	12.520	9.400	14.380	7.700
8	Ce_2O_2	35.050	23.670	29.680	32.320	35.440	23.120
9	Pr_2O_2	0.000	0.610	4.010	4.260	3.670	3.140
10	Nd_2O_3	0.000	1.480	10.930	17.320	13.490	14.850
11	Sm_2O_3	0.000	0.100	1.550	2.290	0.970	4.260
12	Eu_2O_2	0.000	0.000	0.000	0.450	0.000	0.000
13	Gd_2O_3	0.000	0.240	0.940	0.000	0.230	3.450
14	Dy_2O_3	0.000	0.000	0.290	0.110	0.000	0.740
15	Ho_2O_3	0.000	0.000	0.000	0.000	0.160	0.000
16	Er_2O_3	0.000	0.000	0.000	0.090	0.000	0.000
17	Tm_2O_3	0.000	0.000	0.000	0.000	0.130	0.000
18	Yb_2O_3	0.000	0.000	0.110	0.000	0.000	0.000
19	Lu_2O_3	0.000	0.000	0.000	0.000	0.160	0.000
20	P_2O_5	0.000	0.630	0.000	0.000	0.070	0.000
21	MnO	0.200	0.000	0.000	0.140	0.000	0.420
22	MgO	1.900	0.510	0.000	0.210	1.740	0.000
23	SrO	0.000	1.970	0.000	0.000	0.000	0.120
24	CaO	4.480	5.090	7.280	2.220	1.990	8.380
31	BaO	0.450	0.000	0.000	0.000	0.000	0.000
32	Na_2O	0.240	0.000	0.000	0.000	0.000	0.000
33	K_2O	0.160	0.000	0.000	0.000	0.000	0.000
34	S_3O	0.140	0.000	0.000	0.000	0.000	0.000
35	F	0.070	0.000	0.000	1.080	1.850	2.320
36	Cl	0.000	0.000	0.000	0.000	0.050	0.000
37	O=F	0.029	0.000	0.000	0.455	0.779	0.977
38	O=Cl	0.000	0.000	0.000	0.000	0.011	0.000
39	H_2O	2.720	3.200	3.300	1.420	2.500	1.080
40	$\sum$ (wt%)	99.801	98.850	99.150	99.755	99.980	99.523
41	Si	6.981	6.837	7.000	6.986	6.970	6.960
42	Ti	0.019	0.000	0.000	0.000	0.000	0.040
43	Th	0.000	0.000	0.000	0.014	0.012	0.000
44	Al	0.422	0.000	0.698	0.066	0.000	0.699
45	Fe^{3+}	0.217	0.322	0.246	0.681	0.247	0.220
46	Y	0.000	0.000	0.260	0.302	0.028	0.376
47	La	3.478	4.233	1.360	1.029	1.640	0.790
48	Ce	4.028	2.647	3.201	3.510	4.012	2.356
49	Pr	0.000	0.068	0.430	0.460	0.413	0.318
50	Nd	0.000	0.161	1.150	1.835	1.490	1.476
51	Sm	0.000	0.011	0.157	0.234	0.103	0.409
52	Eu	0.000	0.000	0.000	0.046	0.000	0.000
54	Gd	0.000	0.024	0.092	0.000	0.024	0.318
55	Dy	0.000	0.000	0.028	0.011	0.000	0.066
56	Ho	0.000	0.000	0.000	0.000	0.016	0.000
57	Er	0.000	0.000	0.000	0.008	0.000	0.000

Table 3. Continued ...

Row		S1	S2	S3	S4	S5	S6
63	Tm	0.000	0.000	0.000	0.000	0.013	0.000
64	Yb	0.000	0.000	0.010	0.000	0.000	0.000
65	Lu	0.000	0.000	0.000	0.000	0.015	0.000
66	P	0.000	0.163	0.000	0.000	0.018	0.000
67	Mn	0.053	0.000	0.000	0.035	0.000	0.099
68	Mg	0.889	0.232	0.000	0.093	0.802	0.000
69	Sr	0.000	0.349	0.000	0.000	0.000	0.019
70	Ca	1.507	1.666	2.298	0.706	0.659	2.499
71	Ba	0.055	0.000	0.000	0.000	0.000	0.000
72	Na	0.146	0.000	0.000	0.000	0.000	0.000
73	K	0.064	0.000	0.000	0.000	0.000	0.000
74	S	0.033	0.000	0.000	0.000	0.000	0.000
75	∑ (apfu)	17.892	16.714	16.931	16.016	16.461	16.645
76	F	0.069	0.000	0.000	1.013	1.809	2.042
77	Cl	0.000	0.000	0.000	0.000	0.026	0.000
78	OH	5.695	6.521	6.485	2.810	5.156	2.005
79	∑ (apfu)	5.765	6.521	6.485	3.823	6.992	4.047
80	Ca	1.375	1.506	2.298	0.706	0.659	2.499
81	Na	0.000	0.000	0.000	0.000	0.000	0.000
82	Sr	0.000	0.349	0.000	0.000	0.000	0.019
83	K	0.055	0.000	0.000	0.000	0.000	0.000
84	Ba	0.049	0.000	0.000	0.000	0.000	0.000
85	REEY	7.506	7.145	6.689	7.435	7.753	6.110
86	□	0.000	0.000	0.013	0.860	0.587	0.372
87	∑ A-site (apfu)	9.000	9.000	9.000	9.000	9.000	9.000
88	Ca	0.132	0.160	0.000	0.000	0.000	0.000
89	Na	0.146	0.000	0.000	0.000	0.000	0.000
90	Mg	0.291	0.000	0.000	0.000	0.049	0.018
91	□	0.431	0.840	1.000	1.000	0.951	0.982
92	∑ X-site (apfu)	1.000	1.000	1.000	1.000	1.000	1.000
93	Mg	0.598	0.232	0.000	0.093	0.753	0.000
94	Mn	0.053	0.000	0.000	0.035	0.000	0.099
95	Fe^{3+}	0.217	0.322	0.246	0.681	0.247	0.220
96	Al	0.422	0.000	0.698	0.066	0.000	0.699
97	∑ M-site (apfu)	1.291	0.554	0.944	0.875	1.000	1.000
98	Si	6.981	6.837	7.000	6.986	6.970	6.960
99	P	0.000	0.163	0.000	0.000	0.018	0.000
100	Ti	0.019	0.000	0.000	0.000	0.000	0.040
101	Th	0.000	0.000	0.000	0.014	0.012	0.000
102	∑ T-site (apfu)	7.000	7.000	7.000	7.000	7.000	7.000
103	A-site Dominant	Ce	La	Ce	Ce	Ce	Ce
104	X-site Dominant	□	□	□	□	□	□
105	M-site Dominant	Mg	Fe^{3+}	Al	Fe^{3+}	Mg	Al
106	T-site Dominant	Si	Si	Si	Si	Si	Si
107	Z-site Dominant	OH	OH	OH	OH	F	F
108	Group name	CrtG	CrtG	CrtG	CrtG	CrtG	CrtG
109	Subgroup name	CrtSg	CrtSg	CrtSg	CrtSg	TpgSg	TpgSg
110	Species	Crt-Ce	Fecrt-La	Acrt-Ce	Npe-Ce	Tpg-Ce	Atpg-CeCa

Note: (apfu) = Atoms per formula unit. REEY = Rare Earth Elements + Y. □ = vacancy. Samples sources: S1 = from Handbook of Mineralogy (Anthony et al., 2001-2005); S2 = from Pakhomovsky et al. (2002); S3 = from Nestola et al. (2009); S4 = from Allaz et al. (2015); S5 = from Qu et al. (2020); S6 = from Campostrini et al. (2023). CrtG = Cerite group; CrtSg = Cerite subgroup; TpgSg = Taipingite subgroup; Crt-Ce = Cerite-(CeCa), Fecrt-La = Ferricerite-(LaCa), Acrt-Ce = Aluminocerite-(CeCa), Npe-Ce = Nipeiite-(Ce), Tpg-Ce = Taipingite-(CeCa), Atpg-CeCa = Aluminotaipingite-(CeCa). The formulae were recalculated to content of ions on the basis of T-site total = 7.00 (apfu).

Table 4. Chemical compositions of selected merrillite group minerals with calculations and classifications by WinCrtclas.

Row		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
1	SiO_2	0.000	0.000	0.000	0.000	1.160	0.000	0.140	0.000	0.000	0.000
2	TiO_2	0.060	0.000	0.000	0.000	0.070	0.000	0.020	0.000	0.000	0.000
3	Al_2O_3	0.000	0.000	0.000	0.000	0.000	0.250	0.070	0.000	0.000	0.380
4	Cr_2O_3	0.030	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5	Fe_2O_3	0.000	0.000	0.000	0.000	0.000	4.590	0.000	0.000	0.000	0.800
6	Y_2O_3	0.000	0.000	0.000	0.000	0.000	0.000	1.680	0.000	0.000	0.000
7	La_2O_3	0.000	0.000	0.000	0.000	0.000	0.000	0.890	0.000	0.000	0.000
8	Ce_2O_3	0.000	0.000	0.000	0.000	0.050	0.000	2.140	0.000	0.000	0.000
9	Pr_2O_3	0.000	0.000	0.000	0.000	0.000	0.000	0.280	0.000	0.000	0.000
10	Nd_2O_3	0.000	0.000	0.000	0.000	0.210	0.000	1.308	0.000	0.000	0.000
11	Sm_2O_3	0.000	0.000	0.000	0.000	0.000	0.000	0.301	0.000	0.000	0.000
12	Gd_2O_3	0.000	0.000	0.000	0.000	0.000	0.000	0.459	0.000	0.000	0.000
13	Dy_2O_3	0.000	0.000	0.000	0.000	0.000	0.000	0.420	0.000	0.000	0.000
14	Yb_2O_3	0.000	0.000	0.000	0.000	0.100	0.000	0.000	0.000	0.000	0.000
15	V_2O_5	0.000	0.000	0.000	0.000	0.000	0.410	0.000	0.000	0.000	0.000
16	P_2O_5	47.700	45.700	46.240	46.860	43.800	46.110	42.850	46.000	35.200	46.400
17	FeO	0.280	5.200	1.330	1.540	6.070	0.000	6.320	0.000	0.200	0.960
18	MnO	0.000	0.000	0.000	0.000	0.020	0.000	0.110	0.000	0.200	3.700
19	NiO	0.080	0.000	0.000	0.190	0.000	0.000	0.000	0.000	0.000	0.000
20	MgO	3.270	0.900	3.900	4.250	0.000	1.140	0.330	3.610	4.600	0.410
21	SrO	0.000	0.000	0.000	0.310	0.380	0.000	0.000	0.310	51.400	0.910
22	CaO	46.600	47.000	48.870	47.450	48.360	46.400	40.760	46.600	5.500	37.600
23	BaO	0.000	0.000	0.000	0.000	0.000	0.000	0.030	0.000	2.300	0.000
24	Na_2O	2.570	1.400	0.000	0.130	0.000	0.320	0.320	0.460	0.000	5.400
25	K_2O	0.030	0.000	0.000	0.040	0.030	0.100	0.150	0.000	0.000	0.000
26	SO_3	0.000	0.000	0.000	0.000	0.010	0.000	0.000	0.070	0.000	0.000
27	F	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.430	0.000	0.000
28	Cl	0.000	0.000	0.000	0.000	0.020	0.000	0.000	0.000	0.000	0.000
29	O=F	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.181	0.000	0.000
30	O=Cl	0.000	0.000	0.000	0.000	0.005	0.000	0.000	0.000	0.000	0.000
31	H_2O	0.000	0.000	0.000	0.000	0.000	0.250	0.000	0.000	0.000	0.000
32	∑ (wt%)	100.620	100.200	100.340	100.770	100.275	99.570	98.578	97.299	99.400	96.560
33	$H_2O_{Calc.}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.730	0.000	0.736
34	Si	0.000	0.000	0.000	0.000	0.213	0.000	0.027	0.000	0.000	0.000
35	Ti	0.008	0.000	0.000	0.000	0.010	0.000	0.003	0.000	0.000	0.000
36	Al	0.000	0.000	0.000	0.000	0.000	0.053	0.016	0.000	0.000	0.082
37	Cr	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
38	Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.618	0.000	0.000	0.000	0.110
39	Y	0.000	0.000	0.000	0.000	0.000	0.000	0.169	0.000	0.000	0.000
40	La	0.000	0.000	0.000	0.000	0.000	0.000	0.062	0.000	0.000	0.000
41	Ce	0.000	0.000	0.000	0.000	0.003	0.000	0.148	0.000	0.000	0.000
42	Pr	0.000	0.000	0.000	0.000	0.000	0.000	0.019	0.000	0.000	0.000
43	Nd	0.000	0.000	0.000	0.000	0.014	0.000	0.088	0.000	0.000	0.000
44	Sm	0.000	0.000	0.000	0.000	0.000	0.000	0.020	0.000	0.000	0.000
45	Gd	0.000	0.000	0.000	0.000	0.000	0.000	0.029	0.000	0.000	0.000
46	Dy	0.000	0.000	0.000	0.000	0.000	0.000	0.026	0.000	0.000	0.000
47	Yb	0.000	0.000	0.000	0.000	0.006	0.000	0.000	0.000	0.000	0.000
48	V^{5+}	0.000	0.000	0.000	0.000	0.000	0.048	0.000	0.000	0.000	0.000
49	P	7.128	7.029	6.975	7.032	6.807	6.984	6.872	6.934	6.956	7.197
50	Fe^{2+}	0.041	0.790	0.198	0.228	0.932	0.000	1.001	0.000	0.039	0.147
51	Mn	0.000	0.000	0.000	0.000	0.003	0.000	0.018	0.000	0.040	0.574
52	Ni	0.011	0.000	0.000	0.027	0.000	0.000	0.000	0.000	0.000	0.000

Table 4. Continued ...

Row		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
53	Mg	0.860	0.244	1.036	1.123	0.000	0.304	0.093	0.958	1.601	0.112
54	Sr	0.000	0.000	0.000	0.032	0.040	0.000	0.000	0.032	6.957	0.097
55	Ca	8.813	9.148	9.329	9.011	9.513	8.894	8.273	8.891	1.375	7.381
56	Ba	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.210	0.000
57	Na	0.880	0.493	0.000	0.045	0.000	0.111	0.118	0.159	0.000	1.918
58	K	0.007	0.000	0.000	0.009	0.007	0.023	0.036	0.000	0.000	0.000
59	S	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.009	0.000	0.000
60	∑(apfu)	17.753	17.704	17.538	17.507	17.549	17.034	17.021	16.984	17.177	17.618
61	F	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.242	0.000	0.000
62	Cl	0.000	0.000	0.000	0.000	0.006	0.000	0.000	0.000	0.000	0.000
63	OH	0.000	0.000	0.000	0.000	0.000	0.298	0.000	0.867	0.778	0.899
64	∑(apfu)	0.000	0.000	0.000	0.000	0.006	0.298	0.000	1.109	0.778	0.899
65	Ca	8.813	9.000	9.000	8.959	8.930	8.894	8.273	8.891	1.375	7.381
66	Na	0.180	0.000	0.000	0.000	0.000	0.083	0.118	0.077	0.000	1.522
67	Sr	0.000	0.000	0.000	0.032	0.040	0.000	0.000	0.032	6.957	0.097
68	K	0.007	0.000	0.000	0.009	0.007	0.023	0.036	0.000	0.000	0.000
69	Ba	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.210	0.000
70	REEY	0.000	0.000	0.000	0.000	0.023	0.000	0.562	0.000	0.000	0.000
71	□	0.000	0.000	0.000	0.000	0.000	0.000	0.009	0.000	0.457	0.000
72	∑A-site(apfu)	9.000	9.000	9.000	9.000	9.000	9.000	9.000	9.000	9.000	9.000
73	Ca	0.000	0.148	0.329	0.052	0.583	0.000	0.000	0.000	0.000	0.000
74	Na	0.699	0.493	0.000	0.045	0.000	0.028	0.000	0.082	0.000	0.396
75	Fe^{2+}	0.041	0.358	0.198	0.228	0.000	0.000	0.001	0.000	0.039	0.147
76	Mg	0.000	0.000	0.036	0.150	0.000	0.000	0.000	0.000	0.640	0.000
77	□	0.259	0.000	0.437	0.525	0.417	0.972	0.999	0.918	0.321	0.457
78	∑X-site(apfu)	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
79	Fe^{2+}	0.000	0.432	0.000	0.000	0.932	0.000	1.000	0.000	0.000	0.000
80	Mg	0.860	0.244	1.000	0.973	0.000	0.304	0.093	0.958	0.960	0.112
81	Mn	0.000	0.000	0.000	0.000	0.003	0.000	0.018	0.000	0.040	0.574
82	Ni	0.011	0.000	0.000	0.027	0.000	0.000	0.000	0.000	0.000	0.000
83	Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.618	0.000	0.000	0.000	0.110
84	Al	0.000	0.000	0.000	0.000	0.000	0.053	0.016	0.000	0.000	0.082
85	Cr	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
86	∑M-site(apfu)	0.876	0.675	1.000	1.000	0.935	0.975	1.126	0.958	1.000	0.878
87	Si	0.000	0.000	0.000	0.000	0.213	0.000	0.027	0.000	0.000	0.000
88	P	7.128	7.029	6.975	7.032	6.807	6.984	6.872	6.934	6.956	7.197
89	V^{5+}	0.000	0.000	0.000	0.000	0.000	0.048	0.000	0.000	0.000	0.000
90	Ti	0.008	0.000	0.000	0.000	0.010	0.000	0.003	0.000	0.000	0.000
91	∑T-site(apfu)	7.136	7.029	6.975	7.032	7.030	7.032	6.902	6.934	6.956	7.197
92	A-siteDominant	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Sr	Ca
93	X-siteDominant	Na	Na	$Ca_{0.5}□_{0.5}$	$(Fe^{2+})_{0.5}□_{0.5}$	$Ca_{0.5}□_{0.5}$	□	□	□	□	□
94	M-siteDominant	Mg	Fe^{2+}	Mg	Mg	Fe^{2+}	Fe^{3+}	Fe^{2+}	Mg	Mg	Mn
95	T-siteDominant	P	P	P	P	P	P	P	P	P	P
96	Z-siteDominant	□	□	□	□	□	□	□	□	□	□
97	Group	MerG	MerG	MerG	MerG	MerG	MerG	MerG	MerG	MerG	MerG
98	Subgroup	MerSg	MerSg	MerSg	MerSg	MerSg	MerSg	MerSg	WhtSg	WhtSg	WhtSg
99	Species	Mer	Fmer	Kep	Krw	Myh	Dnk	Cgs-Y	Wht	Swht	Wop

Note: (apfu) = Atoms per formula unit. H_2OCalc. = Calculated H_2O (wt%) content based on the stoichiometric constraints by program. □ = Vacancy. Samples sources: S1 = Xie et al. (2003), S2 = from Handbook of Mineralogy (Anthony et al., 2001-2005), S3 = from Britvin et al. (2021), S4 = from Galuskin et al. (2024), S5 = from Hwang et al. (2019), S6 = from Galuskin et al. (2023), S7 = from Yang and Du (2024), S8 = from Hughes et al. (2008), S9 = from Britvin et al. (1991), S10 = from Cooper et al. (2013). MerG = Merrillite group; MerSg = Merrillite subgroup; WhtSg = Whitlockite subgroup; Mer = Merrillite, Fmer = Ferromerrillite, Kep = Keplerite, Krw = Karwowskiite, Myh = Matyhite, Dnk = Deynekoite, Cgs-Y = Changesite-(Y), Wht = Whitlockite, Swht = Strontiowhitlockite, Wop = Wopmayite. The formulae were recalculated to content of ions on the basis of 28 oxygen atoms (apfu).

the output Excel file. The number of ions is calculated on the basis of T-site total=7.00 (apfu) for cerite group minerals and 28 oxygen atoms (apfu) for merrillite group minerals in Tables 3 and 4, respectively. In a case where a chemical composition corresponds to a hitherto unknown species within the cerite supergroup (i.e., a new species), WinCrtclas warns the user with a "Not classified" statement in columns 137, 138, and 139 of the *Calculation Screen* for group, subgroup, and species. For example, a cerite-supergroup mineral with the following analytical data (see Table 4 in Gross et al., 2013; wt%); SiO_2 0.20, Al_2O_3 0.10, P_2O_5 45.93, FeO 1.77, MnO 0.10, MgO 3.19, CaO 46.38, Na_2O 1.36, K_2O 0.06, total 99.09 is defined as merrillite that yields the empirical formula $(Ca_{8.830}Na_{0.157}K_{0.013})_{\sum 9.000}(\square_{0.425}Na_{0.312}Fe^{2+}_{0.263})_{\sum 1.000}$ $(Mg_{0.845}\ Al_{0.021}Mn_{0.015})_{\sum 0.881}(P_{6.909}Si_{0.036})_{\sum 6.944}\square_{\sum 3.000}$ on the basis of 28 oxygen atoms (apfu), where □=vacancy. As can be seen from the empirical formula, calculated content of ions on the basis of 28 oxygen atoms (apfu) indicates that the dominant ions at the A, □, M, T, and Z sites correspond to Ca, □, Mg, P, and □, respectively. As no species corresponding to this composition exists in the current classification scheme (i.e., A=Ca, X=□, M=Mg, T=P, Z=□), the program designates it as 'Not classified' rather than applying the name of one of known species listed in Table 1.

WinCrtclas provides options to display binary and ternary classification and compositional diagrams in the *Calculation Screen* by using the Grapher program. Some of these plots, with selected cerite-supergroup mineral data from the literature, are given in Figure 2. All input and calculated parameters from the *Output* tab of an Excel file (i.e., Output.xlsx) are automatically transposed by the *Transpose* tab of the program. This procedure provides the user with the ability to prepare a quick table for presentation as well as publication by using the *Copy-Paste* option.

SUMMARY AND AVAILABILITY OF THE PROGRAM

WinCrtclas is a user-friendly program that is specially developed for personal computers running on the Windows operating system to estimate and classify the cerite-supergroup minerals using data obtained from both electron-microprobe and wet-chemical analyses. The program processes multiple analytical data sets (up to 200) for each program execution. The current version of WinCrtclas recalculates ions, allocates them into the A, X, M, T, and Z sites, and classifies a total of 17 species for a given analysis into one of two groups (i.e., cerite

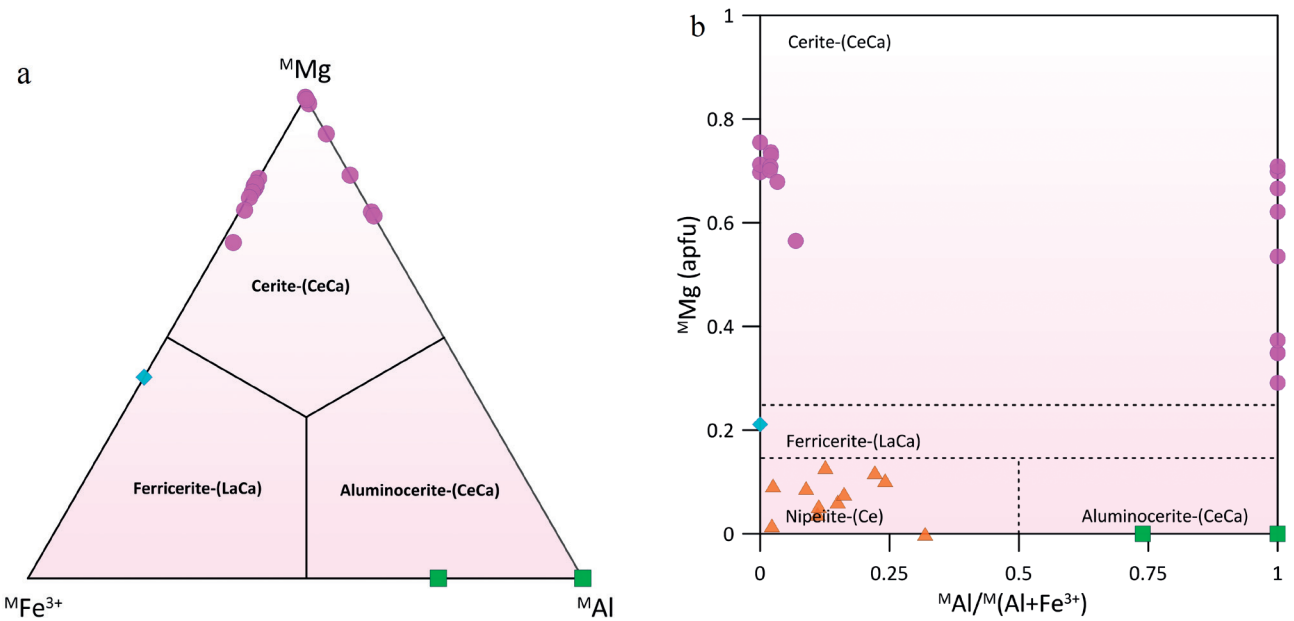

Figure 2 a,b. Selected plots of the cerite-supergroup minerals classification and compositional diagrams from the pull-down menu of *Graph* in the *Calculation Screen* of the WinCrtclas program, using the selected mineral analyses from the literature. a) Compositional plot of the cerite-group minerals in a ternary ^{M}Mg-^{M}Fe^{3+}-^{M}Al diagram, where $^{M}X_i$ shows cation content at the M site [filled diamond from Pakhomovsky et al. (2002); filled circles from Bagiński et al. (2016), Holtstam and Andersson (2007), Turner (2015); filled squares from Förster (2000), Nestola et al. (2009)]. b) Compositional plot of the cerite-group minerals in a ^{M}Al/^{M}(Al+Fe^{3+}) versus Mg diagram, where $^{M}X_i$ shows cation content at the M site [filled diamond from Pakhomovsky et al. (2002); filled circles from Bagiński et al. (2016), Holtstam and Andersson (2007), Turner (2015); filled squares from Förster (2000), Nestola et al. (2009); filled triangles from Allaz et al. (2015)].

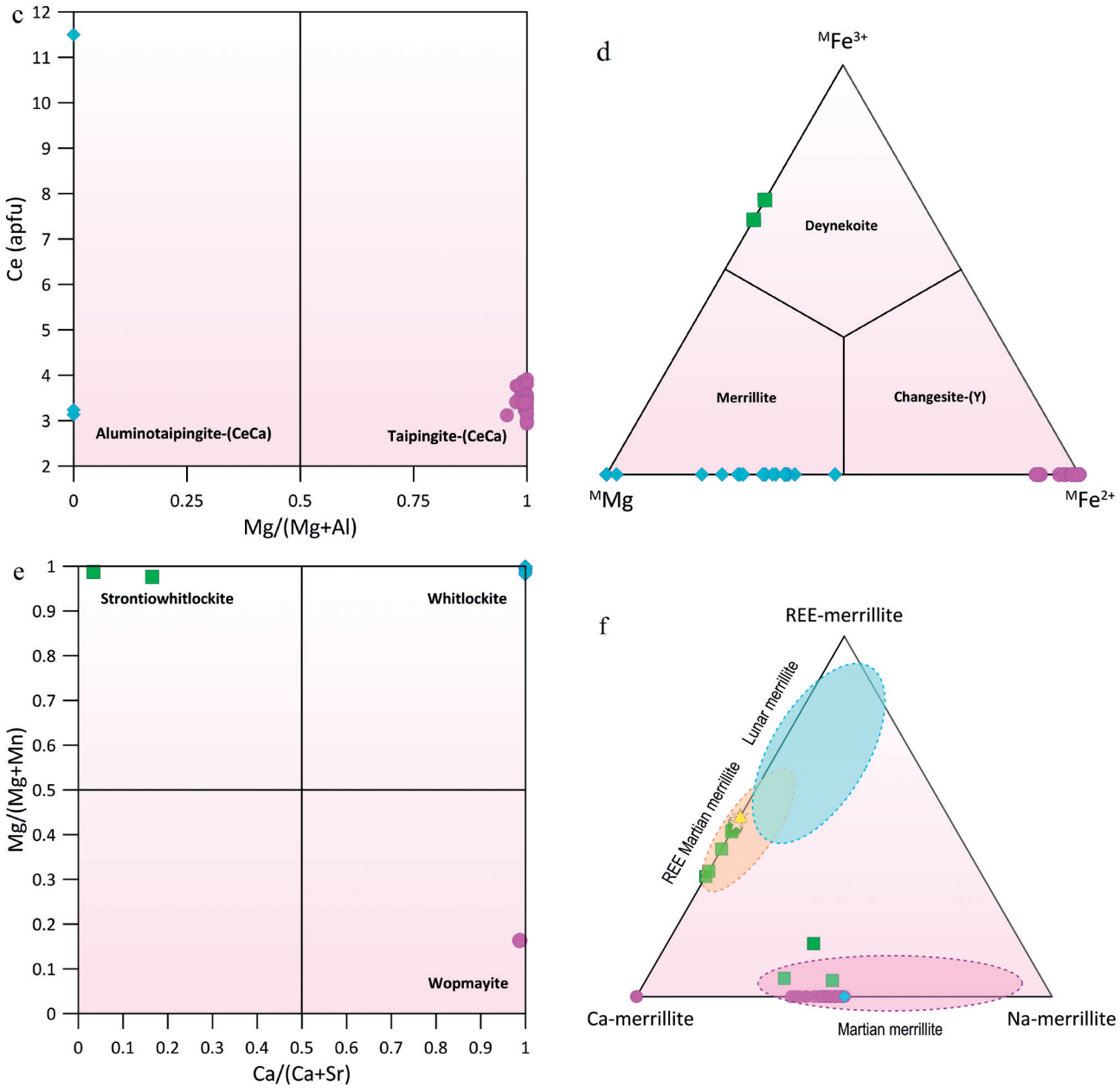

Figure 2 c-f). c) Compositional plot of the cerite-group minerals in a Mg/(Mg+Al) versus Ce diagram [(filled diamonds from Al-Ani and Sarapaa (2000), Förster (2000); filled circles from Holtstam et al. (2007), Qu et al. (2020), Moore and Shen (1983), Hirtopanu et al. (2013)]. d) Compositional plot of the merrillite-group minerals in a ternary $^{M}Fe^{3+}$-^{M}Mg-$^{M}Fe^{2+}$ diagram, where $^{M}X_i$ shows cation content at the M site [filled diamonds from Jolliff et al. (2006), McCubbin et al. (2014), Shearer et al. (2015); filled circles from Yang and Du (2024); filled squares from Galuskin et al. (2023, 2024)]. e) Compositional plot of the merrillite-group minerals in a Ca/(Ca+Sr) versus Mg/(Mg+Mn) diagram [filled diamonds from Jolliff et al. (1993, 2006); filled circles from Cooper et al. (2013); filled squares from Britvin et al. (1991)]. f) Compositional variations of extra-terrestrial merrillites in a ternary REE-merrillite–Ca-merrillite–Na-merrillite diagram (modified from Shearer et al., 2015 and Hwang et al., 2019). [filled diamonds from Jones et al. (2016), filled circles from Ward et al. (2017), filled squares from Shearer et al. (2015), filled triangles from McCubbin et al. (2014), filled stars from Słaby et al. (2017)].

and merrillite) and four subgroups (i.e., cerite, taipingite, merrillite, and whitlockite) using the current IMA-approved nomenclature scheme (Atencio and Azzi, 2020; Atencio et al., 2023). The program generates two main windows. The first window (i.e., *Start-up/Data Entry Screen*), with several pull-down menus and equivalent

shortcuts, enables users to edit a given cerite-supergroup mineral analysis based on chemistry (wt%). By clicking the *Calculate* icon (i.e., ∑) in the *Data Entry Screen*, all input and estimated parameters by WinCrtclas are displayed in the second window (i.e., *Calculation Screen*). The program reports the output in a tabulated form with a numbered column from 1 to 139 in the *Calculation Screen* window, as well as in an Output Excel file. These columns include cerite-supergroup compositions (wt%), recalculated cation and anion values (apfu), contents of ions (apfu) allocated to the sites, dominant anions, groups, subgroups, and species. The results in the *Calculation Screen* can be exported to a Microsoft® Excel file (i.e., Output.xlsx), by clicking the *Send Results to Excel File (Output.xlsx)* icon or selecting the *Send Results to Excel File (Output.xlsx)* option from the pull-down menu of *Excel*. This file is then opened by Excel by clicking the *Open and Edit Excel File (Output.xlsx)* icon or selecting the *Open Excel File (Output.xlsx)* option from the pull-down menu of *Excel*. WinCrtclas is a compiled program that consists of a self-extracting setup file containing all the necessary support files (i.e., "dll" and "ocx") for the 32-bit system. By clicking the setup file, the program and its associated files (i.e., support files, help file, data files with the extension of ".crt", ".xls", ".xlsx" and plot files with the extension of ".grf" are installed into the personal computer (i.e., the directory of C:\Program Files\WinCrtclas or C:\Program Files (x86)\WinCrtclas) on Windows XP and subsequent operating systems. An installation of the program into a personal computer with a 64-bit operating system may require the "msflexgrd" adjustment (see explanations in the Supplementary Material). The self-extracting setup file (i.e., the WinCrtclas setup.exe file) is approximately 14 Mb and can be obtained from the journal's server as a Supplementary Material.

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