

Original paper

# WinSpingc, a Windows program for spinel supergroup minerals

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A Microsoft® Visual Basic software, called WinSpingc, has been developed to calculate and classify wet chemical and electron-microprobe spinel supergroup mineral analyses based on the New Minerals, Nomenclature and Classification (CNMMN) of the International Mineralogical Association (IMA–19) nomenclature scheme. The program evaluates the 60 approved species according to the dominant valence and constituents in the general  $AB_2X_4$  formula for the spinel, ulvöspinel, carrollite, linnaeite, tyrellite and bornhardtite subgroups that belong to the oxyspinel, thiospinel and selenospinel groups. Mineral analyses of the oxyspinel group are calculated based on 3 cations and 4 oxygen atoms per formula unit, whereas the formulae of thiospinel and selenospinel analyses are on the basis of 7 atoms per formula unit. Employing the anions of spinel supergroup mineral analyses, the program first assigns three groups on the basis of dominant X anion, including  $O^{2-}$ ,  $S^{2-}$  and  $Se^{2-}$ , determines subgroups according to the cation charge arrangement combinations and then defines the spinel species in each subgroup based on the dominant valence and constituents. The  $Fe^{3+}$  and  $Fe^{2+}$ , as well as the  $Mn^{3+}$ ,  $Mn^{2+}$ ,  $Co^{3+}$  and  $Co^{2+}$  contents from microprobe-derived total FeO, MnO and CoO (wt. %) amounts, are estimated by stoichiometric constraints. WinSpingc allows the users to enter total 57 input variables for groups as well as to type and load the multiple spinel supergroup compositions in the data entry section, to edit and load the Microsoft® Excel files in calculating, classifying and naming the spinel species, and to store all the calculated parameters in the Microsoft® Excel file for further evaluations. The program is distributed as a self-extracting setup file, including the necessary support files used by the program, a help file, and representative sample data files.

**Keywords:** spinel, oxyspinel, thiospinel, selenospinel, classification, software

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## 1. Introduction

Spinel was one of the first minerals whose structure has been investigated in detail due to its simple structure type that provides incorporation of various monovalent to hexavalent cations, at least 36, within its structure (Bosi 2019). Despite their apparent simplicity, the spinel-type structure presents significant flexibility in cation and anion substitutions due to the interplay between tetrahedral and octahedral sites, which results in approximately five dozen minerals in mainly three oxyspinel, thiospinel and selenospinel groups. Thus, cations partitioning as a function of  $P$ – $T$  conditions, the thermal expansion and the compressibility of the spinel structure are not only the interest for modelling the Earth's mantle, but also subject to a variety of geochemical and petrological applications, including geothermometers, geobarometers and geospeedometers (Biagioni and Pasero 2014; Yavuz and Döner 2017; Yavuz and Yıldırım 2018a; Yavuz 2013, 2021; Yavuz and Yavuz 2022). Besides some spinel species being the source of ore minerals (e.g., chromite for Cr and magnetite for Fe), the others can be used as gemstones (e.g., different colors of spinel species). Minerals with the natural spinel structure are observed in a wide

range of geological (i.e., from the upper mantle to the crust) and extraterrestrial geological environments (e.g., the Moon, Mars, meteorites). On the other hand, materials with the spinel-type structure show different specifications regarding mechanical, optic, thermoelectric and magnetic properties. Hence, natural and synthetic materials with spinel-type structure are suitable for many applications in chemistry and materials science (Bosi 2019).

Most naturally encountered spinel species are oxides (e.g., chromite, magnetite and spinel) when compared to the other more rarely observed sulfides (e.g., carrollite, malanite and grimmite) and selenide (e.g., tyrellite, bornhardtite and trüstedtite) spinel-type minerals. If synthetic compounds in the spinel-type structure were considered, the spinel supergroup expands towards the halides, pseudohalides (cyanides), tellurides and nitrides. Consequently, spinel with  $X = O^{2-}$ ,  $S^{2-}$  and  $Se^{2-}$  in the general formula  $AB_2X_4$  occur in nature, whereas spinel with  $X = F^{1-}$ ,  $Cl^{1-}$ ,  $(CN)^{1-}$ ,  $Te^{2-}$  and  $N^{3-}$  is produced as synthetic phase. Oxide spinels show a large compositional range with primary magmatic and/or secondary origin. The spinel structure consists of a cubic close-packed array of anions (e.g.,  $O^{2-}$ ,  $S^{2-}$ ,  $Se^{2-}$ ) with A (e.g., Cu, Mn, Mg) and B (e.g., Cr, Al, V) constituents occupying

**Tab. 1** A list of the 60 IMA-approved species in the spinel supergroup (from Bosi et al. 2019a) classified by the WinSpingc program

<b>Oxyspinel group</b>					
Row	Spinel subgroup (2-3)	Symbol	A <sup>2+</sup>	B <sup>3+</sup>	X
1	Chihmingite	Cim	Ni	Al <sub>2</sub>	O <sub>4</sub>
2	Chromite	Chr	Fe	Cr <sub>2</sub>	O <sub>4</sub>
3	Chukochenite	Ckc	(Li <sup>+</sup> <sub>0.5</sub> Al <sup>3+</sup> <sub>0.5</sub> )	Al <sub>2</sub>	O <sub>4</sub>
4	Cochromite	Cchr	Co	Cr <sub>2</sub>	O <sub>4</sub>
5	Coulsonite	Cou	Fe	V <sub>2</sub>	O <sub>4</sub>
6	Cuprospinel	Cspl	Cu	Fe <sub>2</sub>	O <sub>4</sub>
7	Dellagiustaite	Dgt	V	Al <sub>2</sub>	O <sub>4</sub>
8	Deltalumite	Dal	(Al <sub>0.67</sub> □ <sub>0.33</sub> )	Al <sub>2</sub>	O <sub>4</sub>
9	Franklinite	Frk	Zn	Fe <sub>2</sub>	O <sub>4</sub>
10	Gahnite	Ghn	Zn	Al <sub>2</sub>	O <sub>4</sub>
11	Galaxite	Glx	Mn	Al <sub>2</sub>	O <sub>4</sub>
12	Guite	Gui	Co	Co <sub>2</sub>	O <sub>4</sub>
13	Hausmannite	Hsm	Mn	Mn <sub>2</sub>	O <sub>4</sub>
14	Hercynite	Hc	Fe	Al <sub>2</sub>	O <sub>4</sub>
15	Hetaerolite	Hta	Zn	Mn <sub>2</sub>	O <sub>4</sub>
16	Jacobsite	Jcb	Mn	Fe <sub>2</sub>	O <sub>4</sub>
17	Maghemite	Mgh	(Fe <sup>3+</sup> <sub>0.67</sub> □ <sub>0.33</sub> )	Fe <sub>2</sub>	O <sub>4</sub>
18	Magnesiochromite	Mchr	Mg	Cr <sub>2</sub>	O <sub>4</sub>
19	Magnesiocoulsonite	Mcou	Mg	V <sub>2</sub>	O <sub>4</sub>
20	Magnesioferrite	Mfr	Mg	Fe <sub>2</sub>	O <sub>4</sub>
21	Magnetite	Mag	Fe	Fe <sub>2</sub>	O <sub>4</sub>
22	Manganochromite	Mnchr	Mn	Cr <sub>2</sub>	O <sub>4</sub>
23	Spinel	Spl	Mg	Al <sub>2</sub>	O <sub>4</sub>
24	Thermaerogenite	Tag	Cu	Al <sub>2</sub>	O <sub>4</sub>
25	Titanomaghemite	Tmgh	(Ti <sup>4+</sup> <sub>0.5</sub> □ <sub>0.5</sub> )	Fe <sub>2</sub>	O <sub>4</sub>
26	Trevorite	Trv	Ni	Fe <sub>2</sub>	O <sub>4</sub>
27	Vuorelainenite	Vuo	Mn	V <sub>2</sub>	O <sub>4</sub>
28	Zincochromite	Zchr	Zn	Cr <sub>2</sub>	O <sub>4</sub>
<i>Ulvöspinel subgroup (4-2)</i>			<b>A<sup>4+</sup></b>	<b>B<sup>2+</sup></b>	<b>X</b>
29	Ahrensitite	Ahr	Si	Fe <sub>2</sub>	O <sub>4</sub>
30	Brunogeierite	Bng	Ge	Fe <sub>2</sub>	O <sub>4</sub>
31	Filipstadite	Fps	(Fe <sup>3+</sup> <sub>0.5</sub> Sb <sup>5+</sup> <sub>0.5</sub> )	Mn <sub>2</sub>	O <sub>4</sub>
32	Qandilite	Qnd	Ti	Mg <sub>2</sub>	O <sub>4</sub>
33	Ringwoodite	Rwd	Si	Mg <sub>2</sub>	O <sub>4</sub>
34	Tegengrenite	Teg	(Mn <sup>3+</sup> <sub>0.5</sub> Sb <sup>5+</sup> <sub>0.5</sub> )	Mg <sub>2</sub>	O <sub>4</sub>
35	Ulvöspinel	Uspl	Ti	Fe <sub>2</sub>	O <sub>4</sub>
<b>Thiospinel group</b>					
<i>Carrollite subgroup (1-3.5)</i>			<b>A<sup>1+</sup></b>	<b>B<sup>3.5+</sup></b>	<b>X</b>
36	Carrollite	Cli	Cu	Co <sub>2</sub>	S <sub>4</sub>
37	Cuproiridsite	Cir	Cu	(Ir <sup>3+</sup> Ir <sup>4+</sup> )	S <sub>4</sub>
38	Cuprokalininite	Ckal	Cu	(Cr <sup>3+</sup> Cr <sup>4+</sup> )	S <sub>4</sub>
39	Fletcherite	Ftc	Cu	Ni <sub>2</sub>	S <sub>4</sub>
40	Florensovite	Frs	Cu	(Cr <sup>3+</sup> <sub>1.5</sub> Sb <sup>5+</sup> <sub>0.5</sub> )	S <sub>4</sub>
41	Malanite	Mla	Cu	(Ir <sup>3+</sup> Pt <sup>4+</sup> )	S <sub>4</sub>
42	Rhodostannite	Rhs	Cu	(Fe <sup>2+</sup> <sub>0.5</sub> Sn <sup>4+</sup> <sub>1.5</sub> )	S <sub>4</sub>
43	Toyohaite	To	Ag	(Fe <sup>2+</sup> <sub>0.5</sub> Sn <sup>4+</sup> <sub>1.5</sub> )	S <sub>4</sub>
<i>Linnaeite subgroup (2-3)</i>			<b>A<sup>2+</sup></b>	<b>B<sup>3+</sup></b>	<b>X</b>
44	Cadmoindite	Cad	Cd	In <sub>2</sub>	S <sub>4</sub>
45	Cuprorhodsite	Crh	(Cu <sup>+</sup> <sub>0.5</sub> Fe <sup>3+</sup> <sub>0.5</sub> )	Rh <sub>2</sub>	S <sub>4</sub>
46	Daubréelite	Dau	Fe	Cr <sub>2</sub>	S <sub>4</sub>
47	Greigite	Grg	Fe	Fe <sub>2</sub>	S <sub>4</sub>
48	Grimmite	Gmm	Ni	Co <sub>2</sub>	S <sub>4</sub>
49	Indite	Idt	Fe	In <sub>2</sub>	S <sub>4</sub>
50	Joegoldsteinite	Jgs	Mn	Cr <sub>2</sub>	S <sub>4</sub>
51	Kalininite	Kal	Zn	Cr <sub>2</sub>	S <sub>4</sub>
52	Linnaeite	Lin	Co	Co <sub>2</sub>	S <sub>4</sub>
53	Polydymite	Pld	Ni	Ni <sub>2</sub>	S <sub>4</sub>
54	Siegenite	Seg	Co	Ni <sub>2</sub>	S <sub>4</sub>
55	Violarite	Vio	Fe	Ni <sub>2</sub>	S <sub>4</sub>
56	Xingzhongite	Xin	Pb	Ir <sub>2</sub>	S <sub>4</sub>
<b>Selenospinel group</b>					
<i>Tyrellite subgroup (1-3.5)</i>			<b>A<sup>1+</sup></b>	<b>B<sup>3.5+</sup></b>	<b>X</b>
57	Nickeltyrellite	Nty	Cu	Ni <sub>2</sub>	Se <sub>4</sub>
58	Tyrellite	Ty	Cu	(Co,Ni) <sub>2</sub>	Se <sub>4</sub>
<i>Bornhardtite subgroup (2-3)</i>			<b>A<sup>2+</sup></b>	<b>B<sup>3+</sup></b>	<b>X</b>
59	Bornhardtite	Bhd	Co	Co <sub>2</sub>	Se <sub>4</sub>
60	Trüstedtite	Trü	Ni	Ni <sub>2</sub>	Se <sub>4</sub>

Symbols from Warr (2021). Chihmingite (Hwang et al. 2022), chukochenite (Rao et al. 2022), grimmite (Škácha et al. 2021) and nickeltyrellite (Förster et al. 2019) are new spinel species approved by the IMA later than the subcommittee report by Bosi et al. (2019a).

one-eighth of the tetrahedrally (i.e., *T*) and one-half of the octahedrally (i.e., *M*) coordinated sites (Bosi 2019). Traditionally, spinels are represented by either “normal”, where the *T* site is occupied by divalent (e.g., Fe<sup>2+</sup>, Mn<sup>2+</sup>, Ni<sup>2+</sup>) cations and the *M* site by trivalent (e.g., Fe<sup>3+</sup>, Mn<sup>3+</sup>, Ni<sup>3+</sup>) cations or “inverse”, where the *T* site is occupied by trivalent cations and the *M* site by one divalent plus one trivalent cation (Bosi et al. 2019a).

Although various computer programs for the calculation and classification of rock-forming silicate minerals have been published over the past two decades (e.g., Yavuz, 2001, 2003, 2007; Yavuz et al. 2014, 2015; Yavuz and Yıldırım 2018b, 2020), software on the classification of spinel supergroup minerals, according to the current IMA report (Bosi et al. 2019a), has not yet been appeared in literature, except for programs specially focused on chromian spinels (Yavuz 1999; Ganuza et al. 2012, 2014; Antonini et al. 2020). In this paper, a computer program, WinSpingc, has been developed using the Microsoft® Visual Basic programming language to calculate multiple spinel supergroup mineral data, up to 200 analyses at a time, obtained from wet chemical and electron-microprobe techniques. The program estimates and classifies oxyspinel group mineral analyses on the basis of 3 cations and 4 oxygen atoms per formula unit “*apfu*”. On the other hand, the formulae of thiospinel and selenospinel analyses were calculated based on “7 *apfu*”. Calculation and classification of spinel supergroup mineral analyses are carried out based on the current IMA report (Bosi et al. 2019a). The program is capable of estimating the FeO, Fe<sub>2</sub>O<sub>3</sub>,

MnO, Mn<sub>2</sub>O<sub>3</sub>, CoO and Co<sub>2</sub>O<sub>3</sub> (wt. %) contents from a microprobe-derived total FeO, MnO and CoO (wt. %) analysis using the stoichiometric constraints proposed by Droop (1987). WinSpingc allows the user to display spinel supergroup minerals in several binary and ternary classification and variation diagrams by using the Golden Software's Grapher program. When compared to the published previous spinel-related computer programs, WinSpingc provides users with a quick evaluation of multiple spinel analyses for calculation and classification purposes according to the current IMA-approved nomenclature scheme by Bosi et al. (2019a).

## 2. Spinel supergroup minerals nomenclature

Considering that mineral nomenclature aims at identifying and naming minerals as well as mineral classification aims at grouping minerals based on their similar properties and reciprocal relations, Bosi et al. (2019b) defined the meaning of mineral formulae and suggested a coherent procedure to identify mineral species based on their formula with contradictions in the current mineral classification scheme. In this respect, the 60 valid minerals of the spinel supergroup have been divided into three groups (i.e., oxyspinel, thiospinel and selenospinel) by Bosi et al. (2019a, see Tab. 1) based on the dominant X species (i.e., anions) in the general AB<sub>2</sub>X<sub>4</sub> formula. In each group, the subdivision procedure into subgroups is carried out according to the cation charge arrangement combinations considering the (A+B) to X atomic ratio of 3:4 (Bosi et al. 2019a). Using this criterion, for example, the oxyspinel group, consisting of 34 species, is divided into the spinel subgroup (2-3) and ulvöspinel subgroup (4-2), where the numbers in parentheses show the charges of cations in A and B (see Tab. 1). According to Bosi et al. (2019a), the subdivision scheme can easily be extended such as subgroups (2-1) and (6-1) if the natural AB<sub>2</sub>X<sub>4</sub> compound with spinel structure is discovered as a new mineral species.

In the spinel classification procedure by a chemical formula, cations at the sites are grouped together and then each species is determined systematically by stoichiometry based on the chemical formula. Bosi et al. (2019a) pointed out that the total variations in spinel composition can easily be described in the ternary system A–B–X, where A and B parameters indicate the greatest degree of variation in terms of cations. However, the system may be reduced to binary A–B if the anion X is specified. As the electroneutrality principle constrains the variation of A and B parameters, only one parameter, the most abundant constituent B in the general formula, is considered to determine the subgroup (Bosi et al. 2019a). Thus, using the recalculated chemical analytical data and considering

the dominant-valency rule, the dominant valence can be determined for the B parameter by summing the ions for each valence. For example, total divalent ( $\sum R^{2+} = \text{Mg}^{2+} + \text{Fe}^{2+} + \text{Mn}^{2+} + \text{Cu}^{2+} + \text{Zn}^{2+} + \text{Co}^{2+} + \text{Ni}^{2+} + \text{V}^{2+}$ ) and trivalent ( $\sum R^{3+} = \text{Cr}^{3+} + \text{Fe}^{3+} + \text{Al}^{3+} + \text{Mn}^{3+} + \text{Co}^{3+}$ ) cations are used to determine the subgroups (2-3) and (4-2) of oxyspinels, which are characterized by  $\sum R^{3+} > 1.0$  “*apfu*” and  $\sum R^{2+} > 1.5$  “*apfu*”, respectively. Bosi et al. (2019a) also stated that the ratio  $\sum R^{3+}/\sum R^{2+}$  can be used to distinguish between the oxyspinels of subgroups (2-3) and (4-2) that can be varying from 0.67 to 2 and 0 to 0.67 values, respectively. Finally, once the valence of B is established, the dominant B-cation and then the dominant A-cation are identified, considering the dominant-constituent rule in which heterovalent pairs of ions also should be taken into account for a proper classification purpose.

Thiospinels and selenospinel (i.e., chalcospinel) are isostructural with oxyspinels, with the anions specified by S<sup>2-</sup> and Se<sup>2-</sup> in the structure, respectively. Although some uncertainties in the ion oxidation states may cause difficulties in the classification of the thiospinel and selenospinel groups and species, they can be divided into the carrollite (1-3.5), linnaeite (2-3), tyrrellite (1-3.5) and bornhardtite (2-3) subgroups (see Tab. 1). Despite chalcospinel have fewer species (i.e., 25) than oxyspinels (i.e., 34), a large number of synthetic spinel structure compounds with S<sup>2-</sup> and Se<sup>2-</sup> have been reported in the literature (Biagioni and Pasero 2014). Albeit the classification of Cu-bearing chalcospinel is more problematic, many of them, including considerable amounts of Cr, Mn, Fe, Co, Ni, Zn, Cd, and In in structure, could be reasonably assigned to subgroup (2-3). According to Bosi et al. (2019a), the charge of ions, for example, in carrollite, fletcherite and tyrrellite, is a matter of discussion. Hence, it is assumed that the oxidation states of anions (i.e., S and Se) and Cu are –2 and +1, respectively. Note that Co<sup>4+</sup> is a result of the S<sup>2-</sup> assumption. Spinel with Co<sup>4+</sup> have not yet been found in nature due to unlikely redox conditions in crustal environments. Thus, the occurrence of cobalt and nickel in Co<sup>3+</sup>, Co<sup>4+</sup>, Ni<sup>3+</sup> and Ni<sup>4+</sup> oxidation states leads to B<sup>3.5+</sup>. Consequently, carrollite, fletcherite and tyrrellite in chalcospinel fall into subgroups (1-3.5).

## 3. Program description

WinSpingc is a user-friendly compiled program package (20 Mb) for spinel supergroup mineral analyses developed for personal computers on the Microsoft® Windows operating system. The program first calculates cations “*apfu*” from electron-microprobe and wet chemical spinel supergroup analyses. Then it classifies the valid 60 species that belong to three groups, including the oxyspinel, thiospinel and selenospinel, within six subgroups

WinSpingc a

File Edit Calculate About Help

*WinSpingc, A Windows Program for Spinel Supergroup Minerals* *Data Entry Screen*

Row No	Sample No [Oxyspinel]	SiO2	TiO2	GeO2	Al2O3	Ti2O3	Cr2O3	V2O3	Fe2O3	Mn2O3	Co2O3	VO	FeO	MgO	CaO	MnO	CuO	ZnO	CoO	NiO	Na2O	K2O	Li2O	Sb2O5
1	Chromite		0.26		9.89		52.17	0.28	5.88				25.48	5.28										
2	Cochromite	0.11	1.26		9.11		50.38		4.14				7.45	0.95		0.84		0.59	17.45	7.67				
3	Coulsonite	0.01	0.22		1.02		24.99	39.98					27.21			2.31		3.79						
4	Cuprospinel				2.6				65.7				1.7	1.8		0.2	27.8	0.7	0.6					
5	Dellagiustalite	0.02	0.73		32.63	0.66		34.88				23.5		7.23		0.41								
6	Deltalunite	0.04			99.74																			
7	Franklinite		0.7		1.25				63.9				3.6			0.6		30.25						
8	Gahnite	0.03			57.71								7.85	0.61		0.65		34.06						
9	Galaxite		0.05		56.3			0.14	4.6						0.83		39.1		0.25					
10	Guite	0.54														0.87	0.73		90.95					
11	Hausmannite												0.01			91.38								
12	Hercynite				60.7								34.7	4.3		0.2								
13	Hetaerolite	0.18							0.24	64.21				0.49		1.86		32.46						
14	Jacobsite		0.38		8.14				59.5				0.5	0.03		32.1								
15	Maghemite	0.3	13		1.8				74.6					8.4		0.9								
16	Magnesiocromite		0.03		17.64		52.33		1.12				16.1	12.13										
17	Magnesiocoulsonite		0.14		0.36		28.09	50.07					0.2	20.90		0.18								
18	Magnesioferrite	0.06			1.63		10.08		67.05				3.15	17.25	0.1	1.01			1.06					
19	Magnetite	0.11	0.29		0.44		0.08		67.16				31.21	0.02		0.09								
20	Manganochromite		0.2				35.9	30.5					5.3			26.3		0.7						
21	Spinel	0.02	0.05		70.08								0.33	28.77				0.33						
22	Thermaerogenite				39.43		0.27		17.96							25.01	17.45							
23	Titanomaghemite	0.68	22.17		1.9				73.26							1.46								
24	Trevorite	1.4							66.24				1.96	0.24					29.71					
25	Vuorelainenite		0.1				19.5	47.4					5.7	0.1		26.4		0.8						
26	Zincochromite	2.82	0.14		1.14		53.3	3.52	2.03									37.05						
27	Chukochente	0.04	0.02		80.7		0.01		8.16					1.7	0.08	2.49		3.25			0.11	0.01	3.68	

WinSpingc b

File Edit Calculate About Help

*WinSpingc, A Windows Program for Spinel Supergroup Minerals* *Data Entry Screen*

Row No	Sample No [Thiospinel]	Cu	Ag	Cd	Fe	Mn	Zn	Ge	Co	Ni	Pb	Bi	Cr	V	In	Sb	As	Sn	Ir	Pd	Pt	Rh	Se	Te	S
1	Carrollite	20.2			0.6				38.6	0.3															41.2
2	Cuproindsite	7.41			3.17					0.27										48.9		10.5	6.05		24.6
3	Cuprokalinite	21.03			0.47		0.17							29.01	5.85		0.08	0.21						43.25	
4	Fletcherite	19.5			0.9				13.6	25.9														41.6	
5	Florensovite	18.8					0.75						24.24	0.02		19.17								38.45	
6	Malanite	9.95			1				2.6	0.33									25.23	0.45	36.77			23.47	
7	Rhodostannite	16			6.8													45.5						31.3	
8	Toyohite	0.14	24.39	0.22	6.28		0.37								0.05			41.24						28.16	
9	Cadmoindite			19.98	1.71		0.77	0.29							49.51									27.53	
10	Cuprorhodsite	7.55			5.31														10.3		6.8	39.6		29.8	
11	Daubreelite				20.1								35.91											42.69	
12	Greigite	0.08			56.5		0.01			0.1			0.14				0.38							42.2	
13	Indite				8.84										59.3									31.85	
14	Joegoldsteinite	0.08			4.5	15.8				0.09			36.2											44.3	
15	Kalinite	2.73					18.89						34.10	0.61		0.73								42.22	
16	Linnaeite	8.79			1.30				40.71	7.35														41.43	
17	Polydymite				3.98				0.63	54.3														41.09	
18	Grimmite	0.08			1.16	0.03			38.23	19.27	0.46	0.62					0.09							41.05	
19	Siegenite	3.16			3.22				20.36	31.24														42.43	
20	Violante	1.12			17.01				1.05	38.68														41.68	
21	Xingzhongite	3.81			1.58						12.8								43.49		9.67	7.19		21.68	

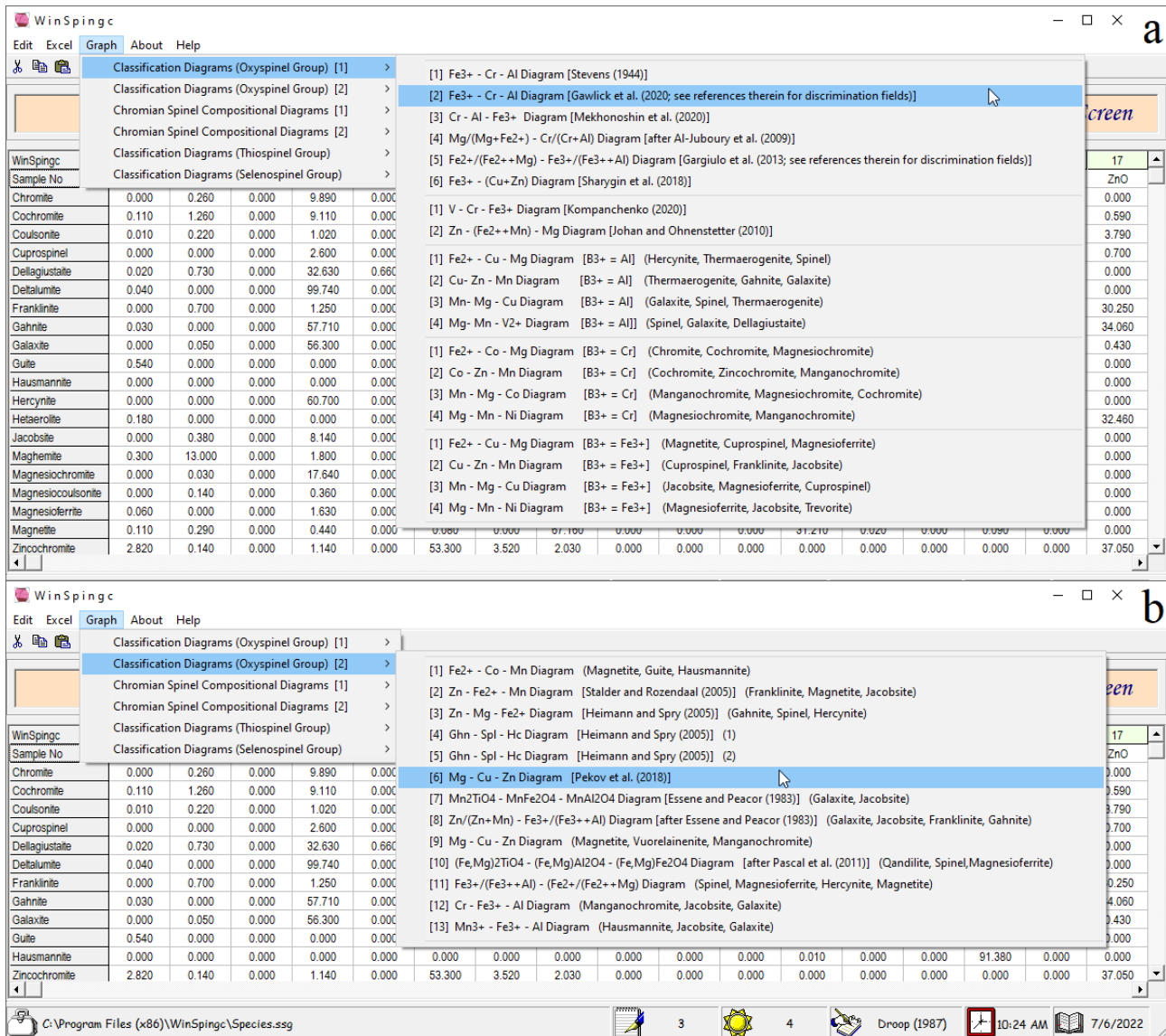
WinSpingc c

File Edit Calculate About Help

*WinSpingc, A Windows Program for Spinel Supergroup Minerals* *Data Entry Screen*

Row No	Sample No [Selenospinel]	Cu	Fe	Co	Ni	Pb	S	Se
1	Tyrrillite	12.7		17.7	6.9			62.4
2	Nicketyrrillite	13.01	0.27	6.66	16.98		1.04	61.91
3	Trüstedite			6.4	29.5			64.4
27								

C:\Program Files (x86)\WinSpingc\Species.ssg 10:24 AM 7/5/2022 by



**Fig. 2a, b** – Screenshots of the binary and ternary classification diagram types for oxyspinels from the pull-down menu of *Graph* in the *Calculation Screen*.

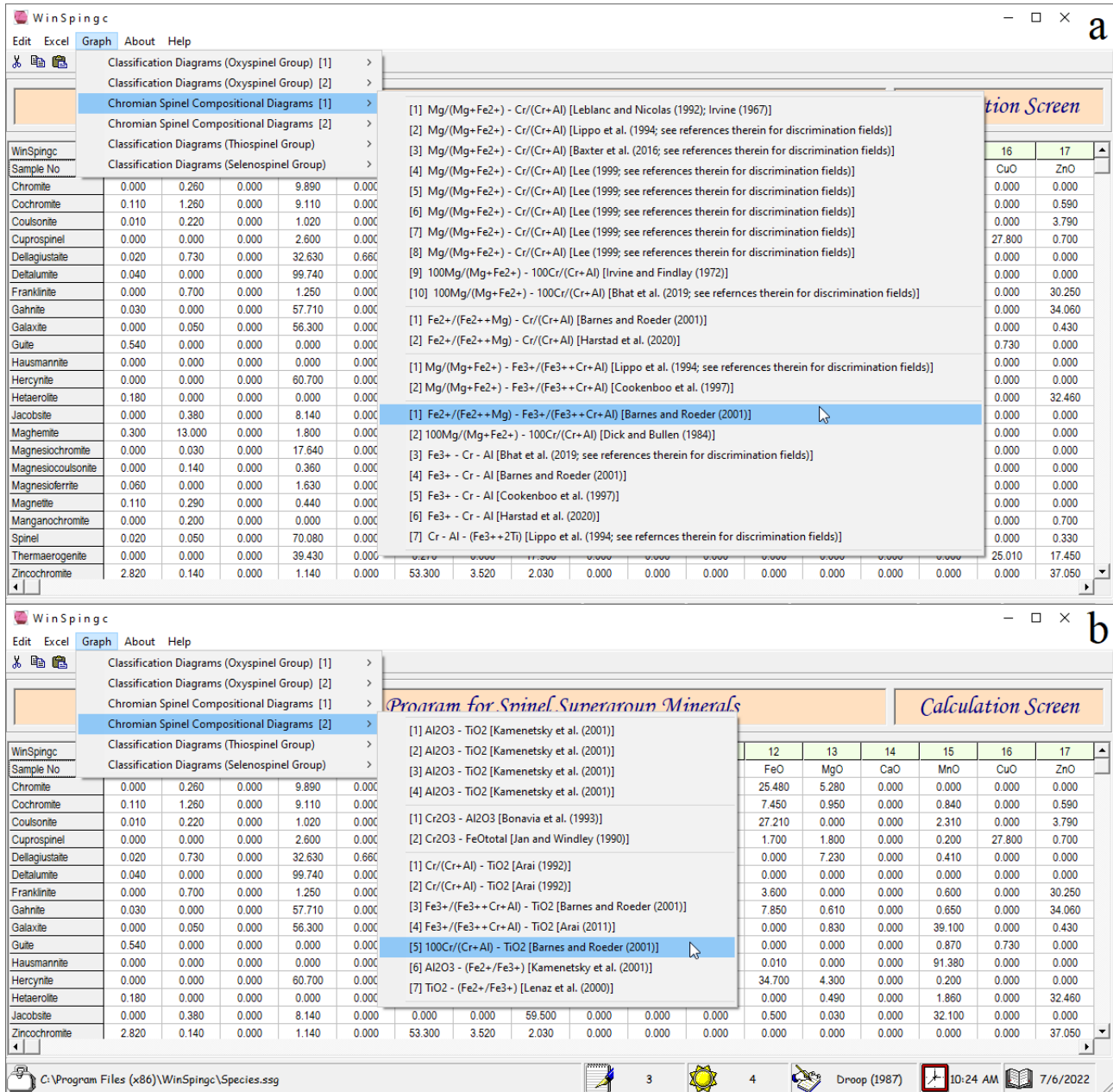
consisting of the spinel (2-3), ulvöspinel (4-2), carrollite (1-3.5), linnaeite (2-3), tyrrellite (1-3.5) and bornhardtite (2-3) (see Tab. 1). A list of the calculation steps in the *Calculation Screen* and an Excel output of the developed program is given in Tab. 2. Current version of WinSpingc presents total 76 binary and ternary classification as well as chromian spinel (Cr-spinel) compositional plots. The Golden Software's Grapher program displays these plots by selecting any diagram type from the pull-down menu of *Graph* in the *Calculation Screen* of WinSpingc.

↩

**Fig. 1** – Screenshots of the WinSpingc *Data Entry Screen* window showing data edit of spinel supergroup minerals. **a** – The standard 23 variables (wt. %) for oxyspinel (wt. %) mineral analyses. **b** – The standard 24 variables for thiospinel (wt. %) mineral analyses. **c** – The standard seven variables for selenospinel (wt. %) mineral analyses.

### 3.1. Data entry of spinel supergroup analyses

Upon successful installation of WinSpingc, the start-up screen with various pull-down menus and equivalent shortcuts appears on the screen. The program allows the user to type wet chemical or electron-microprobe oxyspinel (Fig. 1a), thiospinel (Fig. 1b) and selenospinel (Fig. 1c) analyses both together or as a separate form by clicking the *New* icon on the toolbar, by selecting the *New File* from the pull-down menu of *File* option or pressing the *Ctrl+N* keys. In the *New File*, *Data Entry Screen*, and *Calculation Screen*, these parameters are highlighted by the soft green, pink and blue colors, respectively. WinSpingc uses the standard 57 variables (wt. %) for the calculation and classification of spinel supergroup mineral analyses as in the following orders:



**Fig. 3a, b** – Screenshots of the binary and ternary chromian spinel (Cr-spinel) diagram types from the pull-down menu of *Graph* in the *Calculation Screen*.

Sample No [Oxyspinel],  $\text{SiO}_2$ ,  $\text{TiO}_2$ ,  $\text{GeO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{Ti}_2\text{O}_3$ ,  $\text{Cr}_2\text{O}_3$ ,  $\text{V}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{Mn}_2\text{O}_3$ ,  $\text{Co}_2\text{O}_3$ ,  $\text{VO}$ ,  $\text{FeO}$ ,  $\text{MgO}$ ,  $\text{CaO}$ ,  $\text{MnO}$ ,  $\text{CuO}$ ,  $\text{ZnO}$ ,  $\text{NiO}$ ,  $\text{Na}_2\text{O}$ ,  $\text{K}_2\text{O}$ ,  $\text{Li}_2\text{O}$  and  $\text{Sb}_2\text{O}_5$  (wt. %).

Sample No [Thiospinel],  $\text{Cu}$ ,  $\text{Ag}$ ,  $\text{Cd}$ ,  $\text{Fe}$ ,  $\text{Mn}$ ,  $\text{Zn}$ ,  $\text{Ge}$ ,  $\text{Co}$ ,  $\text{Ni}$ ,  $\text{Pb}$ ,  $\text{Bi}$ ,  $\text{Cr}$ ,  $\text{V}$ ,  $\text{In}$ ,  $\text{Sb}$ ,  $\text{As}$ ,  $\text{Sn}$ ,  $\text{Ir}$ ,  $\text{Pd}$ ,  $\text{Pt}$ ,  $\text{Rh}$ ,  $\text{Se}$ ,  $\text{Te}$ ,  $\text{Se}$  (wt. %).

Sample No [Selenospinel],  $\text{Cu}$ ,  $\text{Fe}$ ,  $\text{Co}$ ,  $\text{Ni}$ ,  $\text{Pb}$ ,  $\text{S}$ ,  $\text{Se}$  (wt. %).

Spinel supergroup analyses typed in an Excel file with the extension of “.xls” and “.xlsx” as in the above 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*, these can be typed in a blank Excel file (i.e., *MySpinel*), 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 *WinSpingc.chm* file on the screen.

### 3.2. Chromian spinel compositional plots

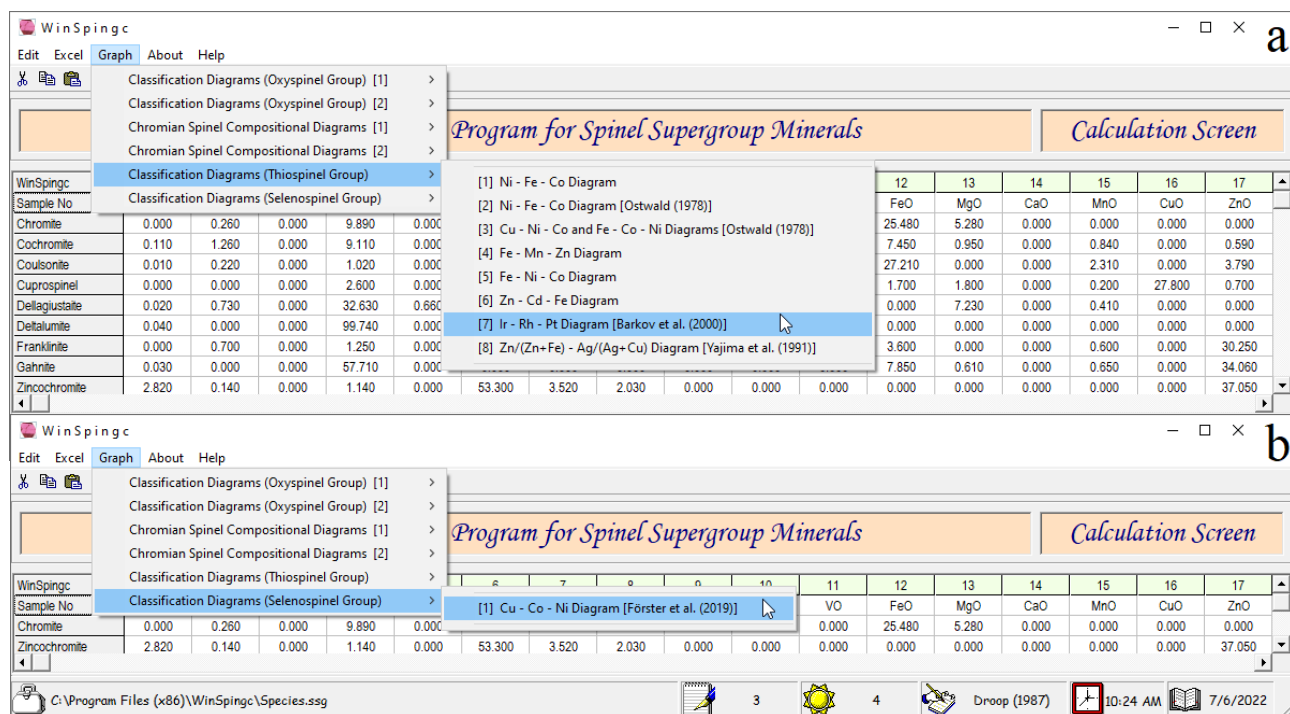
Chromian spinel (Cr-spinel) minerals are important petrogenetic and geochemical indicators crystallizing over a wide range of  $P$ - $T$  conditions in igneous and metamorphic rocks within different geological environments (e.g., Irvine 1965; Dick and Bullen 1984; Barnes and Roeder 2001). Cr-spinel composition has an important role in understanding the upper mantle processes associated with mantle melting and parental melt interactions (Arai et al. 2006). Since the chemical compositions of Cr-spinels were affected by geological factors, including magma composition, sequence of crystallization, oxygen fugacity as well as the  $P$ - $T$  conditions, they also provide Earth scientists with the determination of the different tectonic setting regimes (Dick and Bullen 1984; Sack and Ghiorso 1991; Arai 1992; Barnes and Roeder 2001; Kamenetsky et al. 2001; Arai et al. 2011; Ghosh et al. 2013). Chromite, as a pure end-member of Cr-spinel, in mafic and ultramafic rocks has great economic importance due to the source of chromium ore (Ganuza et al. 2014). Although primary minerals, including olivine and pyroxene in ophiolitic rocks, were subjected to the extensive alteration processes that result in secondary low-temperature minerals such as serpentine and chlorite, the Cr-spinel may be preserved as the primary phase even in completely serpentinized peridotites (Arai 1994a; Bhat et al. 2019). Consequently, the composition of Cr-spinel from mafic and ultramafic rocks is considered in understanding the tectonic setting and petrogenetic processes of host rocks as well as the rate of mid-ocean ridge spreading in numerous earth science studies (e.g., Irvine 1965, 1967; Dick and Bullen 1984; Barnes and Roeder 2001; Kamenetsky et al. 2001; Arai 1992, 1994a, b; Gamal El Dien et al. 2019). However, during low-temperature alteration processes, the chemical composition of primary Cr-spinel may result in a secondary mineral form, called “ferritchromite”, depending on the degree of alteration, but have chemical characteristics that are similar to the primary mantle Cr-spinel compositions (Arai 1978; Arai et al. 2006; Bhat et al. 2019). Cr-spinel, which is found as an accessory mineral in detrital rocks, preserves its compositional signature in buried sedimentary environments due to its mechanical stability; for that reason, it has been used not only in petrogenetic evaluations but also in provenance studies (Lenaz and Princivalle 2005; see references therein). However, Gamal El Dien et al. (2019) demonstrated that the composition of Cr-spinel can be modified by fluid/melt-rock interactions in both sub-arc and sub-mid oceanic mantle environments. Although the Cr# [i.e.,  $\text{Cr}/(\text{Cr}+\text{Al})$ ] of Cr-spinels is an important geochemical parameter for the estimation of the degree of partial melting as well as the provenance of perido-

tites, metasomatism may cause Al-Cr heterogeneity in Cr-spinel composition which lowers the Cr/Al ratio, and therefore changes the Cr#, making Cr# ineffective as a geotectonic and mantle melting indicator (Voigt and von der Handt 2011; Gamal El Dien et al. 2019).

It is common to show spinel supergroup mineral analyses in binary and ternary diagrams for compositional and classification purposes. Some of these plots allow users to determine the spinel species using the cationic values. The current version of WinSpingc enables the users to use a total of 42 visual classification diagrams (e.g., Stevens 1944; Essene and Peacor 1983; Heimann and Spry 2005; Stalder and Rozendaal 2005; Al-Juboury et al. 2009; Johan and Ohnenstetter 2010; Pascal et al. 2011; Gargiulo et al. 2013; Pekov et al. 2018; Sharygin et al. 2018; Gawlick et al. 2020; Kompanchenko 2020; Mekhonoshin et al. 2020) for oxyspinel group compositional data using the Golden Software’s Grapher program. These plots are displayed by selecting the desired diagram type from the pull-down menu of *Graph* in the *Calculation Screen* window of WinSpingc (Fig. 2a, b). Most Cr-spinel-related plots are based on the divalent and trivalent ions for mafic and ultramafic rocks in several geological environments and tectonic settings. The program provides the users total of 34 different plots (e.g., Irvine 1967; Irvine and Findlay 1972; Leblanc and Nicolas 1992; Lippo et al. 1994; Cookenboo et al. 1997; Lee 1999; Barnes and Roeder 2001; Baxter et al. 2016; Harstad et al. 2020) of compositional fields for Cr-spinels (Fig. 3a, b). On the other hand, WinSpingc visually classifies some of the spinel species that belong to the thiospinel and selenospinel groups by selecting the desired diagram type (e.g., Ostwald 1978; Barkov et al. 2000; Yajima et al. 1991; Förster et al. 2019) from the pull-down menu of *Graph* in the *Calculation Screen* window (Fig. 4a, b).

### 4. Worked examples

Using the selected data set from the literature, the following examples show how WinSpingc can be used to estimate and classify the spinel supergroup minerals. Once the previously typed or loaded spinel supergroup analyses are processed by clicking the *Calculate icon* (i.e.  $\Sigma$ ) in the *Data Entry Section* of the program, all input and estimation parameters are displayed in columns 1-163 (see Tab. 2) of the *Calculation Screen* for oxyspinels, thiospinels and selenospinel highlighted by the soft green, pink and blue colors, respectively. 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 “.ssg”. By clicking the *Send results to Excel file* icon in the *Calculation Screen*, all calculations can be stored in



**Fig. 4a, b** – Screenshots of the binary and ternary classification diagram types for thiospinels and selenospinel from the pull-down menu of *Graph* in the *Calculation Screen*.

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

Row	Explanations	Column Numbers
1	Major oxide oxyspinel mineral analyses (wt.%)	1–24
2	Blank	25
3	Recalculated oxyspinel FeO, Fe <sub>2</sub> O <sub>3</sub> , MnO, Mn <sub>2</sub> O <sub>3</sub> , CoO and Co <sub>2</sub> O <sub>3</sub> (wt.%) contents based on the stoichiometric constraints	26–31
4	Blank	32
5	Recalculated cations of oxyspinel mineral analyses “ <i>apfu</i> ”	33–56
6	Blank	57
7	Some useful cation ratio values [e.g., Fe <sup>2+</sup> /(Fe <sup>2+</sup> +Mg), Cr/(Cr+Al)] for Cr–spinel	58–65
8	Blank	66
9	Total divalent to pentavalent cations (i.e., R <sup>2+</sup> , R <sup>3+</sup> , R <sup>4+</sup> , R <sup>5+</sup> ) of oxyspinel mineral analyses “ <i>apfu</i> ”	67–70
10	Blank	71
11	Dominant A and B cations of oxyspinel mineral analyses	72–73
12	Blank	74
13	Group, subgroup and species of oxyspinel mineral analyses	75–77
14	Blank	78
15	Major oxide thiospinel mineral analyses (wt.%)	79–104
16	Blank	105
17	Recalculated cations and anions of thiospinel mineral analyses “ <i>apfu</i> ”	106–130
18	Blank	131
19	Dominant A and B cations of thiospinel mineral analyses	132–133
20	Blank	134
21	Group, subgroup and species of thiospinel mineral analyses	135–137
22	Blank	138
23	Major oxide selenospinel mineral analyses (wt.%)	139–147
24	Blank	148
25	Recalculated cations and anions of selenospinel mineral analyses “ <i>apfu</i> ”	149–156
26	Blank	157
27	Dominant A and B cations of selenospinel mineral analyses	158–159
28	Blank	160
29	Group, subgroup and species of selenospinel mineral analyses	161–163
30	Blank	164

“*apfu*” = Atoms per formula unit; R<sup>2+</sup> = Total divalent cations, R<sup>3+</sup> = Total trivalent cations, R<sup>4+</sup> = Total tetravalent cations, R<sup>5+</sup> = Total pentavalent cations



an Excel file (Output.xlsx) and then displayed by clicking the *Open and edit Excel file* icon.

The validity of program outputs has been tested with representative spinel supergroup mineral analyses (see Tab. 3, Tab. 4, and Tab. 5) selected from literature (e.g., Yajima et al. 1991; Anthony et al. 2001–2005; Cámara et al. 2019; Förster et al. 2019; Kompanchenko 2020; Škácha et al. 2021; Lei et al. 2022). WinSpingc calculates spinel supergroup mineral analyses based on 3 cations and 4 oxygens for oxyspinel group (see rows 31–54 in Tab. 3) and “7 *apfu*” for thiospinel and selenospinel groups (see rows 26–50 in Tab. 4 and rows 9–16 in Tab. 5), respectively.

The program provides the users with some of the useful ratios (see rows 55–62 in Tab. 3), such as  $\text{Fe}^{2+}/(\text{Fe}^{2+}+\text{Mg})$  and  $\text{Cr}/(\text{Cr}+\text{Al})$ , especially for Cr-spinels, in the *Calculation Screen*. Total divalent and trivalent cations, as well as tetra- and pentavalent cations that are used in the classification of oxyspinel mineral analyses are listed (see rows 63–66 in Tab. 3) by the program in the *Calculation Screen*. Similarly, dominant A and B cations with spinel group, subgroup names, and species according to the nomenclature scheme by Bosi et al. (2019a) are also presented in the *Calculation Screen* window for selected spinel supergroup mineral analyses from literature (see rows 67–71 in Tab. 3, rows 51–55 in Tab. 4, rows 17–21 in Tab. 5).

WinSpingc provides various binary and ternary classification and Cr-spinel compositional diagrams in the *Calculation Screen* using Golden Software’s Grapher program. Some of these plots with selected spinel supergroup mineral analyses from literature (e.g., Ostwald 1978; Essene and Peacor 1983; Oktyabrsky et al. 1992; Beard and Tracy 2002; Heimann and Spry 2005; Nekrasov et al. 2005; Beckett-Brown et al. 2018; Harstad et al. 2020) are given in an Electronic Supplementary Material (i.e., ESM 1).

## 5. Summary and availability of the program

WinSpingc is a user-friendly program specially developed for personal computers running on the Windows operating system to estimate and classify the spinel supergroup mineral analyses obtained from electron-microprobe and wet chemical analyses. The program calculates multiple spinel supergroup analyses, up to 200, for each program execution. Following the procedure by Droop (1987), WinSpingc estimates the  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  and, if necessary,  $\text{Mn}^{2+}$ ,  $\text{Mn}^{3+}$ ,  $\text{Co}^{2+}$  and  $\text{Co}^{3+}$  “*apfu*” contents from electron-microprobe oxyspinel analyses using the stoichiometric constraints. The program classifies the 60 valid spinel supergroup minerals into three groups, including oxyspinel, thiospinel and selenospinel based on the current

IMA-approved nomenclature scheme proposed by Bosi et al. (2019a), taking into account the dominant X species in the general  $\text{AB}_2\text{X}_4$  formula.

WinSpingc generates two main windows. The first window (i.e., *Start-up/Data Entry Screen*), with several pull-down menus and equivalent shortcuts, enables to edit spinel supergroup analyses (wt. %). By clicking the *Calculate* icon (i.e.  $\Sigma$ ) in the *Data Entry Screen*, all input and estimated parameters by WinSpingc 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 163 in the *Calculation Screen* window. Calculated oxyspinel, thiospinel and selenospinel parameters, together with the classification subgroups and mineral species, are displayed in 1–77, 80–137, and 140–163 column numbers in the *Calculation Screen*, respectively as well as in an Output Excel file. 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* and then this file is 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*. WinSpingc is a compiled program that consists of a self-extracting setup file including 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 ssg, xls, xlsx and plot files with the extension of grf) are installed into the personal computer (i.e., the directory of C:\Program Files\WinSpingc or C:\Program Files (x86)\WinSpingc) with the Windows XP and later operating systems. An installation of the program into a personal computer with the 64-bit operating system may require the msflexgrd adjustment. This procedure is explained in detail in ESM 2. The self-extracting setup file is 20 Mb and can be obtained from the journal server.

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*Electronic supplementary material.* The supplemental files for the paper are available online at the Journal website (<http://dx.doi.org/10.3190/jgeosci.369>).

Tab. 3 Chemical compositions of selected oxypinel minerals with calculations and classifications by WinSpings

Row	SI	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12
1	SiO <sub>2</sub>	0.01	0.02	0.54	0.00	1.40	0.04	0.00	0.20	0.02	2.98	0.20
2	TiO <sub>2</sub>	0.22	0.73	0.00	0.00	0.00	0.02	0.00	0.00	26.41	1.04	26.30
3	GeO <sub>2</sub>	0.00	0.00	0.00	0.00	0.00	0.00	37.00	0.00	0.00	0.00	0.00
4	Al <sub>2</sub> O <sub>3</sub>	1.02	32.63	0.00	0.00	0.00	80.70	0.00	0.60	4.83	0.35	1.40
5	Ti <sub>2</sub> O <sub>3</sub>	0.00	0.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	Cr <sub>2</sub> O <sub>3</sub>	24.99	0.00	0.00	0.27	0.00	0.01	0.00	0.00	0.00	0.00	0.00
7	V <sub>2</sub> O <sub>3</sub>	39.98	34.88	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20
8	Fe <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	17.96	66.24	8.16	0.00	15.30	28.27	0.17	16.50
9	Mn <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	7.23	0.00
10	Co <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
11	VO	0.00	23.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	FeO	27.21	0.00	0.00	0.00	1.96	0.00	63.80	0.00	10.32	0.00	51.70
13	MgO	0.00	7.23	0.00	0.00	0.24	1.70	0.00	12.30	29.62	23.23	1.80
14	CaO	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00
15	MnO	2.31	0.41	0.87	0.00	0.00	2.49	0.00	36.80	0.76	27.30	0.70
16	CuO	0.00	0.00	0.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	ZnO	3.79	0.00	0.00	0.00	0.00	3.25	0.00	0.00	0.00	1.58	0.00
18	CoO	0.00	0.00	90.95	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	NiO	0.00	0.00	0.00	0.00	29.71	0.00	0.00	0.00	0.00	0.00	0.00
20	Na <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00
21	K <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
22	Li <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	3.68	0.00	0.00	0.00	0.00	0.00
23	Sb <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	34.80	0.00	37.03	0.00
24	Σ (wt.%)	99.59	100.06	99.58	100.12	99.55	100.25	101.76	100.00	100.23	100.91	98.80
25	FeO <sub>calculated</sub>	26.69	0.00	0.00	0.00	0.00	0.00	55.14	0.00	0.00	0.00	0.00
26	Fe <sub>2</sub> O <sub>3</sub> <sub>calculated</sub>	0.58	0.00	0.00	0.00	0.00	0.00	9.63	0.00	0.00	0.00	0.00
27	MnO <sub>calculated</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	Mn <sub>2</sub> O <sub>3</sub> <sub>calculated</sub>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	CoO <sub>calculated</sub>	0.00	0.00	30.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	Co <sub>2</sub> O <sub>3</sub> <sub>calculated</sub>	0.00	0.00	67.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	Si	0.0004	0.0006	0.0217	0.0000	0.0544	0.0010	0.0000	0.0080	0.0006	0.1084	0.0074
32	Ti	0.0062	0.0165	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.5944	0.0285	0.7353
33	Ge	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8540	0.0000	0.0000	0.0000	0.0000
34	Al	0.0447	1.1565	0.0000	0.0000	1.5158	2.3110	0.0000	0.0283	0.1703	0.0150	0.0613
35	Ti <sup>3+</sup>	0.0000	0.0166	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36	Cr	0.7345	0.0000	0.0000	0.0070	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
37	V <sup>3+</sup>	1.1916	0.8410	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0060
38	Fe <sup>3+</sup>	0.0162	0.0000	0.0000	0.4408	1.9385	0.1492	0.2913	0.4614	0.6364	0.0047	0.4614

Tab. 3 Continued

Row	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12
39	Mn <sup>3+</sup>	0.0000	0.0000	2.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2002	0.0000
40	Co <sup>3+</sup>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41	V <sup>2+</sup>	0.0000	0.6343	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	Fe <sup>2+</sup>	0.8298	0.0000	0.0000	0.0000	0.0637	0.0000	1.8544	0.0000	0.2582	0.0000	1.6068
43	Mg	0.0000	0.3241	0.0000	0.0000	0.0139	0.0616	0.0000	0.7349	1.3209	1.2596	0.0997
44	Ca	0.0000	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000
45	Mn	0.0727	0.0104	0.0296	0.0000	0.0000	0.0512	0.0000	1.2492	0.0193	0.8410	0.0220
46	Cu	0.0000	0.0000	0.0221	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47	Zn	0.1040	0.0000	0.0000	0.0000	0.4202	0.0000	0.0583	0.0000	0.0000	0.0424	0.0000
48	Co <sup>2+</sup>	0.0000	0.0000	0.9700	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49	Ni	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	Na	0.0000	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.0000	0.0000	0.0000	0.0000
51	K	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
52	Li	0.0000	0.0000	0.0000	0.0000	0.0000	0.3596	0.0000	0.0000	0.0000	0.0000	0.0000
53	Sb <sup>5+</sup>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5181	0.0000	0.5003	0.0000
54	∑ "apfir"	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000
55	Fe <sup>3+</sup> /Fe <sup>2+</sup>	0.02	0.00	0.00	0.00	30.41	0.00	0.16	0.00	2.46	0.00	0.29
56	Fe <sup>3+</sup> /(Fe <sup>3+</sup> +Fe <sup>2+</sup> )	0.02	0.00	0.00	0.00	0.97	1.00	0.14	1.00	0.71	1.00	0.22
57	Cr/(Cr+Al)	0.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
58	Fe <sup>2+</sup> /(Fe <sup>2+</sup> +Mg)	1.00	0.00	0.00	0.00	0.82	0.00	1.00	0.00	0.16	0.00	0.94
59	Cr/(Cr+Al+Fe <sup>3+</sup> )	0.92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
60	Fe <sup>3+</sup> /(Fe <sup>3+</sup> +Al+Cr)	0.02	0.00	0.00	0.22	1.00	0.06	1.00	0.94	0.79	0.24	0.88
61	Al/(Al+Fe <sup>3+</sup> +Cr)	0.06	1.00	0.00	0.77	0.00	0.94	0.00	0.06	0.21	0.76	0.12
62	Ti/(Ti+Cr+Al)	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.78	0.65	0.92
63	∑ R <sup>2+</sup>	1.01	0.97	1.02	1.00	1.01	0.17	1.85	1.98	1.60	2.14	1.73
64	∑ R <sup>3+</sup>	1.99	2.01	1.96	2.00	1.94	2.46	0.29	0.49	0.81	0.22	0.53
65	∑ R <sup>4+</sup>	0.01	0.02	0.02	0.00	0.05	0.00	0.85	0.01	0.59	0.14	0.74
66	∑ R <sup>5+</sup>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.52	0.00	0.50	0.00
67	Dominant A cation	Fe <sup>2+</sup>	V <sup>2+</sup>	Co <sup>2+</sup>	Mn <sup>2+</sup>	Ni <sup>2+</sup>	Li <sub>0.5</sub> Al <sub>0.5</sub>	Ge <sup>4+</sup>	(Fe <sup>3+</sup> ) <sub>0.5</sub> (Sb <sup>5+</sup> ) <sub>0.5</sub>	Ti <sup>4+</sup>	(Mn <sup>3+</sup> ) <sub>0.5</sub> (Sb <sup>5+</sup> ) <sub>0.5</sub>	Ti <sup>4+</sup>
68	Dominant B cation	V <sup>3+</sup>	Al <sup>3+</sup>	Co <sup>3+</sup>	Mn <sup>3+</sup>	Fe <sup>3+</sup>	Al <sup>3+</sup>	Fe <sup>2+</sup>	Mn <sup>2+</sup>	Mg <sup>2+</sup>	Mg <sup>2+</sup>	Fe <sup>2+</sup>
69	Spinel Group	Oxy	Oxy	Oxy	Oxy	Oxy	Oxy	Oxy	Oxy	Oxy	Oxy	Oxy
70	Spinel Subgroup	(3-2)	(3-2)	(3-2)	(3-2)	(3-2)	(3-2)	(4-2)	(4-2)	(4-2)	(4-2)	(4-2)
71	Spinel Species	Cou	Dgt	Gui	Hsm	Trv	Ckc	Bng	Fps	Qnd	Teg	Uspl

Samples of S1 = from Kompanchenko (2020), S2 = from Cámara et al. (2019), S3 = from Let et al. (2022), S4, S5, S6, S8, S10, S11 and 12 = from Handbook of Mineralogy (Anthony et al. 2001–2005), S7 = from Rao et al. (2022), S9 = from Dunn et al. (1988); The formulae were recalculated to 3 cations and 4 oxygens; Calculated oxides in rows 25 to 30 from total FeO, MnO and CoO (wt.%) contents were carried out on the basis of stoichiometric constraints using the Droop's (1987) method; "apfir" = Atoms per formula unit; R<sup>2+</sup> = Total divalent cations, R<sup>3+</sup> = Total trivalent cations, R<sup>4+</sup> = Total tetravalent cations, R<sup>5+</sup> = Total pentavalent cations; Oxy = Oxyspinel; (3-2) = Spinel subgroup; (4-2) = Ulvöspinel subgroup; Cou = Coulsomite, Dgt = Dellagustaita, Gui = Guite, Hsm = Hausmannite, Tag = Thermanogenite, Trv = Trevorite, Ckc = Chukochenite, Bng = Brunogerite, Fps = Filipstadite, Qnd = Qandilite, Teg = Tegengrenite, Uspl = Ulvöspinel.

Tab. 4 Chemical compositions of selected thiospinel minerals with calculations and classifications by WinSpinge

Row	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12
1	Cu	20.20	21.03	9.95	0.14	0.00	0.08	8.79	0.00	0.08	3.16	3.81
2	Ag	0.00	0.00	0.00	24.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	Cd	0.00	0.00	0.00	0.22	19.98	0.00	0.00	0.00	0.00	0.00	0.00
4	Fe	0.60	0.47	1.00	6.28	1.71	4.50	1.30	3.98	1.16	3.22	1.58
5	Mn	0.00	0.00	0.00	0.00	0.00	15.80	0.00	0.00	0.03	0.00	0.00
6	Zn	0.00	0.17	0.00	0.37	0.77	0.00	0.00	0.00	0.00	0.00	0.00
7	Ge	0.00	0.00	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.00	0.00
8	Co	38.60	0.00	2.60	0.00	0.00	0.00	40.71	0.63	38.23	20.36	0.00
9	Ni	0.30	0.00	0.33	0.00	0.00	0.09	7.35	54.30	19.27	31.24	0.00
10	Pb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.46	0.00	12.80
11	Bi	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00
12	Cr	0.00	29.01	0.00	0.00	35.91	36.20	0.00	0.00	0.00	0.00	0.00
13	V	0.00	5.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	In	0.00	0.00	0.00	0.05	49.51	0.00	0.00	0.00	0.00	0.00	0.00
15	Sb	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	As	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00
17	Sn	0.00	0.00	0.00	41.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	Ir	0.00	0.00	25.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	43.49
19	Pd	0.00	0.00	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	Pt	0.00	0.00	36.77	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9.67
21	Rh	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.19
22	Se	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	Te	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	S	41.20	43.25	23.47	28.16	27.53	44.30	41.43	41.09	41.05	42.43	21.68
25	Σ (%)	100.90	100.07	99.80	100.85	99.79	100.97	99.58	100.00	100.99	100.41	100.22
26	Cu	0.9900	0.9810	0.8560	0.0100	0.0000	0.0040	0.4280	0.0000	0.0040	0.1500	0.3550
27	Ag	0.0000	0.0000	0.0000	1.0300	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	Cd	0.0000	0.0000	0.0000	0.0090	0.8280	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	Fe	0.0330	0.0250	0.0980	0.5120	0.1430	0.2330	0.0720	0.2220	0.0650	0.1740	0.1670
30	Mn	0.0000	0.0000	0.0000	0.0000	0.0000	0.8330	0.0000	0.0000	0.0020	0.0000	0.0000
31	Zn	0.0000	0.0080	0.0000	0.0260	0.0550	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32	Ge	0.0000	0.0000	0.0000	0.0000	0.0190	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33	Co	2.0390	0.0000	0.2410	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34	Ni	0.0160	0.0000	0.0310	0.0000	0.0000	0.0040	2.1390	0.0330	2.0270	1.0440	0.0000
35	Pb	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3880	2.8880	1.0260	1.6090	0.0000
36	Bi	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0070	0.0000	0.3650
37	Cr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0090	0.0000	0.0000
38	V	0.0000	1.6550	0.0000	0.0000	0.0000	2.0160	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.3410	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

39	In	0.0000	0.0000	0.0000	0.0020	2.0090	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40	Sb	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41	As	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0040	0.0000	0.0000
42	Sn	0.0000	0.0000	0.0000	1.5820	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43	Ir	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3390
44	Pd	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45	Pt	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2930
46	Rh	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4130
47	Se	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48	Te	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49	S	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000
50	Σ "apfu"	7.0800	7.0200	7.0000	7.1700	7.0500	7.1600	7.0900	7.0300	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400	7.1400
51	Dominant A cation	Cu	Cu	Cu	Ag	Cd	Fe	Mn	Co	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Pb
52	Dominant B cation	Co	(Cr <sup>3+</sup> Cr <sup>4+</sup> )	(Ir <sup>3+</sup> Pt <sup>4+</sup> ) (Fe <sup>2+</sup> ) <sub>0.5</sub> (Sn <sup>4+</sup> ) <sub>1.5</sub>	Thio	In	Cr	Cr	Co	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ni	Ir
53	Spinel Group	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio	Thio
54	Spinel Subgroup	(1-3.5)	(1-3.5)	(1-3.5)	(1-3.5)	(1-3.5)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)	(2-3)
55	Spinel Species	Cli	Ckal	Mla	To	Cad	Dau	Jgs	Lin	Pld	Pld	Pld	Pld	Pld	Pld	Pld	Pld	Pld	Pld	Pld	Pld	Xin

Samples of S1, S2, S3, S5, S6, S7, S8, S9, S11 and S12 = from Handbook of Mineralogy (Anthony et al. 2001–2005), S4 = from Yajima et al. (1991), S10 = from Škacha et al. (2021); The formulae were recalculated based on 7 "apfu"; Thio = Thiospinel; (1-3.5) = Carrollite subgroup; (2-3) = Linnacite subgroup; Cli = Carrolite, Ckal = Cuprokalinitite, Mla = Malanite, To = Toyohaitite, Cad = Cadmoindite, Dau = Daubréchite, Jgs = Joergelsteinite, Lin = Linnacite, Pld = Polydymite, Gmm = Grimmitite, Seg = Stegenite, Xin = Xingzhongite.

**Tab. 5** Chemical compositions of selected selenospinel minerals with calculations and classifications by WinSpinge

Row		S1	S2	S3
1	Cu	12.70	13.01	0.00
2	Fe	0.00	0.27	0.00
3	Co	17.70	6.66	6.40
4	Ni	6.90	16.98	29.50
5	Pb	0.00	0.00	0.00
6	S	0.00	1.04	0.00
7	Se	62.40	61.91	64.40
8	Σ (%)	99.70	99.87	100.30
9	Cu	1.0120	1.0440	0.0000
10	Fe	0.0000	0.0250	0.0000
11	Co	1.5200	0.5770	0.5330
12	Ni	0.5950	1.4760	2.4650
13	Pb	0.0000	0.0000	0.0000
14	S	0.0000	0.1650	0.0000
15	Se	4.0000	4.0000	4.0000
16	Σ "apfu"	7.1300	7.2900	7.0000
17	Dominant A cation	Cu	Cu	Ni
18	Dominant B cation	Co, Ni	Ni	Ni
19	Spinel Group	Seleno	Seleno	Seleno
20	Spinel Subgroup	(1-3.5)	(1-3.5)	(2-3)
21	Spinel Species	Ty	Nty	Trü

Samples of S1 and S3 = from Handbook of Mineralogy (Anthony et al. 2001–2005), S2 = from Förster et al. (2019); The formulae were recalculated based on 7 atoms per formula unit ("apfu"); Seleno = Selenospinel; (1-3.5) = Tyrrellite subgroup; (2-3) = Bornhardtite subgroup; Ty = Tyrrellite, Nty = Nickeltyrrellite, Trü = Trüstedite.

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