Refractive Indices of Minerals and Synthetic Compounds

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Abstract

This is a comprehensive compilation of refractive indices of 1933 minerals and 1019 synthetic compounds including exact chemical compositions and references taken from 30 compilations and many mineral and synthetic oxide descriptions. It represents a subset of about 4000 entries used by Shannon and Fischer (Amer. Mineral. 101, 2016, 2288-2300) to determine the polarizabilities of 270 cations and anions after removing 425 minerals and compounds containing the lone-pair ions (Tl^{+}, Sn^{2+}, Pb^{2+}, As^{3+}, Sb^{3+},Bi^{3+}, S^{4+}, Se^{4+}, Te^{4+}, Cl^{5+}, Br^{5+}, I^{5+}) and uranyl ions, U^{6+}. The table lists the empirical composition of the mineral or synthetic compound, the ideal composition of the mineral, the mineral name or synthetic compound, the Dana classes and subclasses extended to include beryllates, aluminates, gallates, germanates, niobates, tantalates, molybdates, tungstates, etc., descriptive notes, e.g. structure polytypes and other

information that helps define a particular mineral sample, and the locality of a mineral when known. Finally, we list n_x, n_y, n_z, $<n_{Dobs}>$ (all determined at 589.3 nm), $<n_{Dcalc}>$, deviation of observed and calculated mean refractive indices, molar volume V_m, corresponding to the volume of one formula unit, anion molar volume V_{an}, calculated from V_m divided by the number of anions (O^{2-}, F^-, Cl^-, OH^-) and H_2O in the formula unit, the total polarizability $<\alpha_{AE}>$, and finally the reference to the refractive indices for all 2952 entries. The total polarizability of a mineral, $<\alpha_{AE}>$, is a useful property that reflects its composition, crystal structure, and chemistry and was calculated using the Anderson-Eggleton relationship $\alpha_{AE} = \frac{(n_D^2-1)V_m}{4\pi+\left(\frac{4\pi}{3}-c\right)(n_D^2-1)}$ where $c = 2.26$ is the electron overlap factor. The empirical polarizabilities and therefore, the combination of refractive indices, compositions, and molar volumes of the minerals and synthetic oxides in the table were verified by a comparison of observed and calculated total polarizabilities, $<\alpha_{AE}>$ derived from individual polarizabilities of cations and anions. The deviation between observed and calculated refractive indices is less than 2% in most instances.

Keywords: Refractive index, electronic polarizabilities, optical properties, minerals, synthetic compounds, refractive-index calculation, Anderson-Eggleton relationship.

Introduction

The most important optical properties of minerals and synthetic materials include, along with absorption, their refractive indices (Nesse, 2013). Although identification of minerals by the refractive index measurement has been replaced by the use of electron microprobes (EMP), scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM-EDX), X-ray fluorescence spectroscopy (XRF), X-ray diffraction (XRD), Infrared spectroscopy (IR), and Raman spectroscopy, the refractive index still provides important mineral information and can be used for rapid identification of most common minerals using tables and charts (Feklichev, 1992).

As stated in Shannon and Fischer (2016), refractive indices are also used to predict optical properties from chemical compositions, which is of value in developing new materials, particularly borate optical crystals (Qin and Li, 2011). The refractive index is also an important parameter of lasers and is required, for instance, in the analysis of the radiative properties of Ln^{3+} ions (Han et al., 2012).

Refractive indices can be used to characterize chemical variations in a mineral, much as X-ray powder patterns can help understand chemical trends in structural families, illustrated in the studies of andalusites, adularia, cordierites and zeolites (Bloss et al. 1983; Gunter and Bloss, 1982; Selkregg and Bloss, 1980; Gunter and Ribbe, 1993; Palmer and Gunter, 2000). They can also help determine H_2O content of hydrated minerals and zeolites (Gunter and Ribbe, 1993). Considering the importance of optical properties, especially in mineralogy, it is of particular interest to estimate and predict refractive indices from chemical compositions and crystal-structure parameters. This is possible using the polarizabilities of the ions as listed by Shannon and Fischer (2006) for infinite wavelengths and by Shannon and Fischer (2016) for λ=589.3 nm as described in detail below (see section on calculation of refractive indices). Furthermore, in conjunction with calculated refractive indices using empirical polarizabilities, the refractive indices reflect the composition, crystal structure, valence state, and bond valences of the ions in the crystal (Shannon and Fischer, 2006, 2016).

However, to the best of our knowledge most of the RI compilations provide only “generic” values without inclusion of the specific compositions, unit cells, or mineral locality for specific values of RI's. Generic refractive index values are only approximations when solid solutions involving ions of greatly differing polarizabilities are present. For example in the solid solution series pyrope ($Mg_3Al_2Si_3O_{12}$) - knorringite ($Mg_3Cr_2Si_3O_{12}$), RI = 1.83 ± 0.01 for pure knorringite (Ringwood, 1977) as shown in Figure 1, whereas RI = 1.803 for knorringite from Basutoland, South Africa, with the composition $Mg_{1.90}Ca_{0.66}Fe_{0.41}Mn_{0.17}Cr_{1.04}Al_{0.86}Fe_{0.07}Si_3O_{12}$ (Nixon and Hornung, 1968). Similarly, in the solid solution series tephroite (Mn_2SiO_4) - (γ- Ca_2SiO_4), RI = 1.772, 1.804, and 1.814 for pure tephroite, Mn_2SiO_4, (Greer, 1932) as shown in Figure 2, whereas RI = 1.761, 1.787, and 1.799 for tephroite from Pajsberg, Värmland, Sweden, with the composition $Mn_{1.85}Mg_{0.15}SiO_4$ (Shannon et al., 2002). In the rare cases of minerals observed with ideal stoiochiometric compositions the generic RI is valid. This paper remedies most of those shortcomings by providing observed and calculated RI values along with total polarizabilities, unit cells, compositions, and mineral localities for a large number of minerals and synthetic compounds.

Data Base

There are many sources of refractive index data. Most provide only the refractive indices with no information on (1) the specific composition and unit-cell dimensions associated with the RI, (2) the mineral locality, or (3) a journal reference to the data. Table 1 summarizes the information in some important compilations of optical properties.

The following sources were used: Handbook of Mineralogy (Anthony et al., 2015); Dana's New Mineralogy, (Gaines et al., 1997); The Microscopic Determination of the Nonopaque Minerals (Larsen, 1921); Die oxydischen Kristallphasen der anorganischen Industrieprodukte (Trojer, 1963); Mineralogy Database (Webmineral, 2015); Landolt-Börnstein

(Hellwege and Hellwege, 1962, 1969, 1979, 1981); Rock-forming Minerals (Deer, Howie, and Zussman, 1963a, 1963b, 1978, 1982, 1986, 1996). The volumes by Deer, Howie, and Zussman provide RI, composition, source, and reference with unit cells given for cubic compounds such as garnets but not other families such as olivines, pyroxenes, tourmalines, or humites, although references given there can sometimes be found with unit cell information.

Information on synthetic compounds is generally more complete than on minerals because the stoichimetry is known. See for example: Standard X-ray Diffraction Patterns, NBS Circular 539 and Monograph 25, Sections 1 - 18 (Swanson et al., 1962-1981); The Microscopic Characters of Artificial Inorganic Solid Substances or Artificial Minerals (Winchell, 1931; Winchell and Winchell, 1964); and Handbook of Laser Science and Technology (Weber,1986,1995). In these references, the RI, composition, and unit cells are given but not usually the associated journal references.

The data necessary for this compilation are the refractive indices, crystal structure, unit-cell dimensions, and chemical composition. Refractive indices were taken from the publications listed in Table 1, which includes Palache et al. (1944, 1951, 1962); Gaines et al. (1997); Deer, Howie, and Zussman (1963a, 1963b, 1978, 1982, 1986, 1996); Anthony et al. (2015); Hintze (1897, 1915, 1933, 1938, 1960, 1968); Hellwege and Hellwege (1962, 1969, 1979, 1981); Nelson (1996); McLune (1989); Medenbach and Shannon (1997); Shannon et al. (2002); Shannon and Fischer, (2016); Swanson et al. (1962-1981); Webmineral (2015); Winchell (1931); Winchell and Winchell (1964). They were also taken from the powder diffraction files of the International Centre for Diffraction Data (ICDD) and descriptions of minerals in mineralogical journals. In general the above publications were used to locate the refractive indices and the original publications. Original publications were preferred in order to provide refractive indices, crystal structure, unit-cell dimensions, and chemical composition on the same sample. Occasionally, unit-cell dimensions and composition were taken from the Inorganic Crystal Structure Database (Belsky et al. 2002).

The complete data set consisted of approximately 4000 refractive index measurements on 3000 minerals and 1000 synthetic compounds, ~275 F-containing compounds, 85 Cl-containing compounds, and 700 hydroxyl-containing compounds. The data set contains 400 silicates, 120 carbonates, 20 nitrates,~ 375 sulfates, and 15 perchlorates. [Table S1 in the supplements[1] shows a total of 2952 data on minerals and synthetic compounds]. Some data were not included for various reasons. These are summarized in Table 3 of Shannon and Fischer (2016) and include, with a few examples:

1. Poor or no analysis – composition uncertain: taikanite (Armbruster et al., 1993); cerchiaraite-Mn (Basso et al., 2000);
2. Analysis total < 100%: e.g., haineaultite (McDonald and Chao, 2004);
3. Rare earth ions not specified: e.g., thalenite (Fitzpatrick and Pabst, 1986);
4. Iron valence uncertain - Fe^{2+}/Fe^{3+}: e.g., morimotoite (Henmi et al., 1995);
5. H_2O content uncertain: e.g., hydroandradite (Peters, 1965);
6. Zonation: e.g., morimotoite (Henmi et al., 1995); londonite (Simmons et al., 2001); Zn sonolite (Cook, 1969);
7. Only two indices measured (common): e.g., liebenbergite (DeWaal and Calk, 1973); mercallite (Carobbi, 1935); and
8. Crystal reacts with immersion fluid: e.g., millosevichite (Miura et al., 1994).

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[1] Deposit item AM-xx-xxxxx, Supplemental Table. Deposit items are free to all readers and found on the MSA web site, via the specific issue's Table of Contents (go to http://www.minsocam.org/msa/ammin/toc/2017/...).

Compounds containing lone-pair ions (Tl^{+}, Sn^{2+}, Pb^{2+}, As^{3+}, Sb^{3+},Bi^{3+}, S^{4+}, Se^{4+}, Te^{4+}, Cl^{5+}, Br^{5+}, I^{5+}) and uranyl ions, U^{6+} (~425 compounds) showing systematic deviations between observed and calculated RI's were not included in the database (Shannon and Fischer, 2016) as well as compounds with duplicate RI measurements (~650 compounds).

Special cases include (1) 35 compounds with corner-shared octahedral (CSO) network and chain structures, (2) 40 compounds containing edge-sharing Fe^{3+} and Mn^{3+} octahedra (ESO) such as $LiFeO_2$ and goethite (FeOOH), (3) 40 alkali ion conductors, and (4) 120 sterically-strained (SS) structures with strong bond valence deviations (Shannon and Fischer, 2016). Although these ~235 compounds show large deviations of observed to calculated polarizabilities, they, nevertheless, have excellent optical data included in Table S1.

Calculation of refractive indices

Refractive indices are calculated using the polarizabilities of cations and anions compiled in Shannon and Fischer (2016). The cation polarizabilities are simply additive. The anion polarizabilities are calculated using the relationship

$$\alpha_{-} = \alpha_{-}^{o} \cdot 10^{-N_o/V_{an}^{n}} \qquad (1)$$

with α_{-} = anion polarizability, α_{-}^{o} = free-ion polarizability, and V_{an} = anion molar volume (calculated from the molar volume V_m divided by the number of O^{2-}, F^{-}, Cl^{-}, OH^{-}, and H_2O in the formula unit) as described by Shannon and Fischer (2006). However, the exponent n of the anion volume was empirically determined to yield the best results for $n = 1.2$ (see Shannon and Fischer, 2016). The α_{-}^{o} and N_o parameters are listed in Table 5 in Shannon and Fischer (2016). Summing cation and anion polarizabilities yields the total polarizability of a compound. As an example, the total polarizability of orthoclase, $KAlSi_3O_8$, is calculated according to α(K) + α(Al)

+ 3×α(Si) + 8×α(O) = $1.35 + 0.533 + 3 \cdot 0.284 + 8 \cdot 1.79 \cdot 10^{-1.776/22.51^{1.2}}$ = 15.724 Å^3. In a classical approach, also used by Shannon and Fischer (2006), the mean refractive index can be calculated from the total polarizability using the Lorenz-Lorentz relationship solved for n

$$\alpha_{LL} = \frac{1}{b} V_m \cdot \frac{n^2 - 1}{n^2 + 2} \qquad (2)$$

with the Lorentz factor $b = 4\pi/3$, V_m = molar volume in Å^3, and n = the mean refractive index. In Shannon and Fischer (2016), and thus also here, we are using a relationship modified by Anderson (1975) and Eggleton (1991)

$$\alpha_{AE} = \frac{(n^2-1)V_m}{4\pi + \left(\frac{4\pi}{3} - c\right)(n^2-1)} \qquad (3)$$

with the electronic overlap factor empirically determined to be c = 2.26. This equation solved for the refractive index n yields

$$n_{AE} = \sqrt{\frac{4\pi\alpha_{AE}}{(c-b)\alpha_{AE} + V_m} + 1} \qquad (4)$$

Using V_m = 180.10 Å^3 and the total polarizability calculated above for albite yields the mean refractive index <n> = 1.523 in excellent agreement with the experimentally determined value of 1.524 (see albite entries in Table S1).

Results

This study lists the database of minerals and synthetic compounds used to calculate the empirical polarizabilities by Shannon and Fischer (2016). Minerals are frequently classified using the Strunz or Dana systems (Mills et al. 2009). We have chosen to sort the minerals and synthetics using the Dana classification in Dana's New Mineralogy (Gaines et al. (1997) and Dana's classes/subclasses with Borates as an example: Borates/Class 24: Anhydrous Borates; Class 25:

Anhydrous Borates containing Hydroxyl or Halogen; Class 26: Hydrated Borates containing Hydroxl or Halogen and Class 27: Compound Borates.

Table 2 summarizes information on selected oxide and hydroxide minerals or compounds, where, with the exceptions of compounds showing steric strain and having edge-, face-shared, and corner-shared octahedra, the mean deviation $\Delta = ((<n_D>obs - <n_D>calc)/ <n_D>obs) = 0.7\%$. In column 1 we list the empirical composition of the mineral or synthetic compound. In column 2 we list the mineral or compound name. Column 3 lists the locality of a mineral when known or whether the compound was prepared synthetically. Columns 4-13 list n_x, n_y , n_z, $<n_D>_{obs}$, $<n_D>_{calc}$, Δ, V_m, V_{an} ,$<\alpha_{AE}>$, and reference. In column 12 we list the total polarizability of a mineral, α_{AE}, a useful property that reflects its composition, crystal structure, and chemistry (Shannon and Fischer, 2016).

In some cases, the cation sums in their respective crystallographic sites did not correspond to the ideal or refined values of the sums of cations found from the structure analysis. In many of those minerals (approximately 35 out of the total of ~ 2000 minerals) the cation composition was normalized to agree with the structure analysis identified as "normalized" in column 5 ("Notes" section) of Table 2.

Table 3 summarizes the compositions found by chemical analysis and the normalized composition for 6 silicates, 5 phosphates, 1 arsenate, and 2 sulfate minerals. Normalized cation compositions generally did not differ by more than 5% from the chemical analytical value. Normalization generally improved the fit between α(obs) and α(calc).

Table S1 (Supplementary data[1]) contains the most important information in this work and represents about 20 years of data compilation. It summarizes the total data set of minerals and synthetic compounds. In column A we list the empirical composition of the mineral or synthetic compound. In general, we preferred to use the empirical composition listed in the formal mineral description, e.g. $Na_{2.06}K_{0.95}(Y_{0.77}Dy_{0.09}Gd_{0.04}Er_{0.04}Ho_{0.02}Sm_{0.02}Nd_{0.01}Tb_{0.01})Si_6O_{15}$ (moskvinite-Y; Sokolova et al., 2003). Occasionally, when the empirical composition was not available, we used the composition found in structure analyses, although these compositions are sometimes idealized, e.g. $Na_2KY(Si_6O_{15})$ (see moskvinite-Y; ICSD 97289).

In general, integral numbers of H_2O molecules were used in the compilation and calculations of polarizabilities. In some instances non-integral numbers were used. In column B we list the ideal mineral composition. In column C we list the mineral or compound name. In columns D and E we list the Dana categories. Column F contains descriptive notes, e.g. structure polytypes, sample numbers from Deer, Howie, and Zussman, and other information that helps define a particular mineral sample. Column G lists the locality of a mineral when known or whether the compound was prepared synthetically. Columns H-S list n_x, n_y , n_z, $\langle n_D\rangle_{obs}$,$\langle n_D\rangle_{calc}$, Δn, deviation (%), remarks, V_m, V_{an}, and $\langle \alpha_{AE}\rangle$, where V_m = molar volume in Å^3 corresponding to the volume of one formula unit, V_{an} = anion molar volume , and $\langle \alpha_{AE}\rangle$ is the mean total polarizability calculated from the individual polarizabilities of the ions as described above. Columns T-X contain the refractive index reference.

Figure 3 shows statistical data on the distribution of deviations between observed and calculated refractive indices. It clearly demonstrates that the majority of deviations is in the range below 1 % for 2,377 entries. Another 370 entries have deviations below 2 %.

Implications

The comprehensive table presented here provides a set of accurate refractive index, composition, unit cell volume, and locality data for 1800 minerals and 1030 synthetic compounds arranged according to Dana's classification scheme. The table can serve as a primary source of optical data for mineralogists, chemists, and physicists. It thus represents a large database compiled during the last 20 years used to calculate the empirical polarizabilities of cations and anions by regression analyses. The scheme of calculating total polarizabilities and hence refractive indices using the Anderson-Eggleton relationship will be a powerful tool to predict refractive indices.

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Figure captions:

Figure 1. Refractive indices of pyrope-knorringite solid solutions $Mg_3(Al_{1-x}Cr_x)_2Si_3O_{12}$. Lattice parameter of knorringite from Novak and Gibbs (1971), *a* = 11.64 Å (α(Al) = 0.47 Å^3, α(Cr) = 3.02 Å^3), the line is calculated from polarizabilities, points are from Ringwood (1977).

Figure 2. Refractive indices of tephroite-γ- Ca_2SiO_4 series $(Mn_xCa_{1-x})_2SiO_4$ (Greer, 1932) (α(Ca) = 1.79 Å^3, α(Mn) = 2.07 Å^3).

Figure 3. Frequency of occurrence of absolute values of deviations between observed and calculated refractive indices $\left|\frac{n_{obs}-n_{calc}}{n_{obs}}\right| \cdot 100$ in Table S1 (supplementary data[1]) in the range from 0 % to 3 %, excluding entries with systematic deviations as indicated in the remarks column of Table S1.

549 **Table 1.** Refractive index compilations

Refractive-index sources	Information provided	Reference
Dana's New Mineralogy, The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana,	RI, uc, location [no specific composition, uc or reference]	Gaines et al., (1997); Dana's New Mineralogy;
Empirical electronic polarizabilities in oxides, hydroxides, oxyfluorides, and oxychlorides	RI, composition, uc, references	Shannon and Fischer (2006); minerals and synthetics.
Empirical electronic polarizabilities of ions for the prediction and interpretation of refractive indices	RI, composition, uc, references	Shannon and Fischer (2016); minerals and synthetics.
Handbook of Mineralogy	RI, uc, composition, location, references;	Anthony (2015); Handbook of Mineralogy: www.handbookofmineralogy.org;
Handbook of Optical Materials	RI, composition, references [uc from ICSD or JCPDS]	Weber, CRC Handbook of Laser Science and Technology (1986, 1995); synthetics.
International Critical Tables of Numerical Data, Physics, Chemistry and Technology	RI, references [uc from ICSD or JCPDS]	Washburn (1930) International Critical Tables of Numerical Data, Physics, Chemistry and Technology –synthetics and minerals.
Landolt-Börnstein	RI, references [no uc or mineral location].	Hellwege, K.N., and Hellwege, A.M. (1962-

		1981) Landolt-Börnstein.
Microscopic Characters of Artificial Inorganic Solid Substances or Artificial Minerals	RI, composition, symmetry [uc from ICSD or JCPDS]	Winchell (1931); Winchell and Winchell (1964) synthetics.
Mineralogy Database	RI, composition, uc, location[no specific composition, uc or reference]	Mineralogy Database: Webmineral.com.
NBS Circular and Monograph Series	synthetics - RI, composition, uc	NBS Circular 539 (1955-1960) Standard X-ray Diffraction Patterns; Monograph Series 25 (1962-1981) Standard X-ray Diffraction Patterns- Sections 1-15.
Oxydischen Kristallphasen der anorganischen Industrieproduckte	synthetics and minerals- RI,uc, references	Trojer – Die oxydischen Kristallphasen der anorganischen Industrieprodukte (1963);
Refractive index and dispersion of fluorides and oxides.	RI, composition, uc, references	Shannon and Fischer (2002); minerals and synthetics.
Rock-Forming Minerals.	minerals, RI, composition, location, references, [no uc]	Deer, Howie and Zussman (1963-1996);
System of Mineralogy	RI, composition, uc, locations [no specific	Palache, Berman and Frondel (1944,

	composition, uc or reference]	1952,1962) Dana's system of mineralogy, minerals.
USGS Bulletin 1627	RI [no composition or location]	Fleischer et al. (1984) USGS Bulletin 1627.

Notes: RI = refractive index; uc = unit cell

Table 2. Information on selected oxide and hydroxide minerals or compounds, where, with the exceptions of compounds showing steric strain, and having edge-, face-shared, and corner-shared octahedra, the mean deviation, $\Delta = ((\langle n_D \rangle obs - \langle n_D \rangle calc) / \langle n_D \rangle obs) = 0.7\%$.

Measured chemical formula	Compound name	Locality	n_x	n_y	n_z	$\langle n_D \rangle$	$\langle n_D \rangle$ calc	Δ [%]	V_m	V_{ox}	$\langle \alpha_{AE} \rangle$	Reference
H_2O	ice		1.3091	1.3091	1.3105	1.3096	1.300	0.4	32.58	32.58	1.648	Shannon et al. (2002)
Cu_2O	cuprite		2.849	2.849	2.849	2.849	2.856	-0.2	38.84	38.84	10.513	Palache et al. (1944)
BeO	bromellite	Synthetic	1.7184	1.7184	1.7342	1.7237	1.726	-0.1	13.79	13.79	1.661	Shannon et al. (2002)
MgO	periclase	Synthetic	1.7355	1.7355	1.7355	1.7355	1.719	0.9	18.67	18.67	2.284	Shannon et al. (2002)
CaO	lime	Synthetic	1.8396	1.8396	1.8396	1.8396	1.745	5.0[a]	27.83	27.83	3.865	Shannon et al. (2002)
SrO		Synthetic	1.871	1.871	1.871	1.871	1.786	4.5[a]	33.16	33.16	4.768	Pynchon and Sieckmann (1966)
BaO		Synthetic	1.9841	1.9841	1.9841	1.9841	1.764	11.1[a]	42.48	42.48	6.843	Anderson and Hensley (1975)
ZnO	zincite	Synthetic	2.0222	2.0222	2.0256	2.0233	1.862	8.0[a]	23.55	23.55	3.931	Bond (1965)
HgO	montroydite	Terlingua, Texas	2.37	2.5	2.65	2.5067	2.551	-1.8	32.13	32.13	7.459	Palache et al. (1944)
B_2O_3		Synthetic	1.653	1.653	1.632	1.646	1.636	0.6	45.26	15.09	4.877	Burianek et al. (2016)
Al_2O_3	corundum		1.7673	1.7673	1.7598	1.7648	1.776	-0.6	42.45	14.15	5.393	Shannon et al. (2002)
$Fe_{1.98}Fe_{0.02}O_3$	hematite	Elba Island, Livorno, Tuscany, Italy	3.19	3.19	2.912	3.0973	2.620	15.5[b]	50.32	16.77	14.839	Shannon et al. (2002)
Sc_2O_3		Synthetic	1.9943	1.9943	1.9943	1.9943	1.965	1.5	59.64	19.88	9.698	Shannon et al. (2002)
Y_2O_3		Synthetic	1.9311	1.9311	1.9311	1.9311	1.858	3.8[b]	74.5	24.83	11.403	Shannon et al. (2002)
Eu_2O_3		Synthetic	1.969	1.969	1.969	1.969	1.970	0.0	80.05	26.68	12.713	Shannon et al. (2002)

Gd_2O_3		Synthetic	1.977	1.977	1.977	1.977	1.964	0.6	79.01	26.34	12.643	Ruchkin et al. (1967)
Dy_2O_3		Synthetic	1.9757	1.9757	1.9757	1.9757	1.959	0.8	75.86	25.29	12.124	Shannon et al. (2002)
Ho_2O_3		Synthetic	1.963	1.963	1.963	1.963	1.995	0.4	74.57	24.86	11.775	Ruchkin et al. (1967)
Er_2O_3		Synthetic	1.959	1.959	1.959	1.959	1.954	0.3	73.33	24.44	11.535	Shannon et al. (2002)
Tm_2O_3		Synthetic	1.951	1.951	1.951	1.951	1.943	0.4	72.07	24.02	11.249	Ruchkin et al. (1967)
Yb_2O_3		Synthetic	1.9468	1.9468	1.9468	1.9468	1.934	0.6	70.98	23.66	11.034	Shannon et al. (2002)
Lu_2O_3		Synthetic	1.9349	1.9349	1.9349	1.9349	1.935	0.0	70.1	23.37	10.77	Shannon et al. (2002)
SiO_2	coesite	Synthetic	1.594	1.5955	1.599	1.5962	1.598	-0.1	34.17	17.08	3.401	Sclar et al. (1962)
SiO_2	cristobalite		1.487	1.487	1.484	1.486	1.496	-0.7	42.33	21.16	3.433	Gaines et al. (1997)
SiO_2	quartz	Zambia	1.5444	1.5444	1.5535	1.5474	1.550	-0.2	37.66	18.83	3.442	Shannon et al. (2002)
SiO_2	quartz	Para, Brazil	1.5444	1.5444	1.5533	1.5474	1.550	-0.2	37.66	18.83	3.442	Shannon et al. (2002)
SiO_2	quartz	Synthetic	1.5442	1.5442	1.5533	1.5472	1.550	-0.2	37.66	18.83	3.441	Shannon et al. (2002)
SiO_2	stishovite	Synthetic	1.799	1.799	1.826	1.808	1.800	0.4	23.25	11.62	3.114	Anthony et al. (2016)
SiO_2	tridymite	Plumas County, California	1.478	1.479	1.481	1.4793	1.486	-0.4	43.4	21.7	3.471	Durrell (1940)
SiO_2	SiO_2-keatite	Synthetic	1.522	1.522	1.513	1.519	1.521	-0.2	40.02	20.01	3.468	Keat (1954)
SiO_2	silicalite	Synthetic	1.39	1.39	1.39	1.39	1.391	-0.1	55.27	27.63	3.586	Flanigen et al. (1978)
TiO_2	anatase	Binnental, Switzerland	2.5621	2.5621	2.4889	2.5377	2.561	-0.9	34.07	17.03	8.038	Shannon et al. (2002)
TiO_2	anatase	Binnental, Switzerland	2.5608	2.5608	2.4879	2.5365	2.561	-1.0	34.07	17.03	8.033	Shannon et al. (2002)
TiO_2	brookite	Virgental, Tyrol, Austria	2.585	2.584	2.702	2.6237	2.667	-1.6	32.3	16.1	7.947	Shannon et al. (2002)
TiO_2	rutile	Synthetic	2.6098	2.6098	2.8976	2.7057	2.741	-1.3	31.21	15.61	7.968	Rams et al. (1997)

$Zr_{0.94}Hf_{0.02}Ca_{0.02}Ti_{0.02}O_2$	baddeleyite	Phaloaborwa, South Africa	2.136	2.236	2.243	2.205	2.247	-1.9	35.22	17.61	6.796	Hiemstra (1955)
$Zr_{0.671}Y_{0.329}O_{1.835}$		Synthetic	2.0691	2.0691	2.0691	2.0691	2.137	-3.3^{d}	34.46	18.78	5.984	Shannon et al. (2002)
$Zr_{0.869}Y_{0.131}O_{1.934}$		Synthetic	2.1581	2.1581	2.1581	2.1581	2.229	-3.3^{d}	33.86	17.51	6.312	Shannon et al. (2002)
GeO_2		Synthetic	1.695	1.695	1.735	1.7083	1.720	-0.7	40.5	20.25	4.776	Laubengayer and Morton (1932)
GeO_2		Synthetic	1.96	1.96	2.048	1.9893	2.017	-1.4	27.62	13.81	4.471	Shannon et al. (2002)
SnO_2	cassiterite	Araca, Bolivia	2.0004	2.0004	2.0971	2.0326	2.040	-0.4	35.77	17.87	6.02	Hellwege and Hellwege (1962)
HfO_2		Synthetic	2.06	2.1	2.14	2.1	2.115	-0.7	34.55	17.27	6.154	Gavrish et al. (1975)
$Hf_{0.85}Y_{0.15}O_{1.925}$		Synthetic	2.0881	2.0881	2.0881	2.0881	2.106	-0.9	33.9	17.61	5.98	Shannon et al. (2002)
CeO_2		Synthetic	2.425	2.425	2.425	2.425	2.765	-14.0^{a}	39.71	19.86	8.818	Gavrish et al. (1975)
P_2O_5		Synthetic	1.545	1.578	1.589	1.5707	1.573	-0.2	81.84	16.37	7.798	Hill et al. (1944)
V_2O_5	shcherbinaite	Synthetic	2.89	2.1	2.55	2.5133	2.000	20.3^{c}	89.52	17.9	20.856	King and Suber (1955)
$MoO_3 \cdot 2H_2O$	sidwillite	Lake Como, Colorado	1.7	2.21	2.38	2.0967	1.734	19.3^{c}	95.94	19.19	17.044	Cesbron and Ginderow (1985)
WO_3		Synthetic	2.703	2.376	2.282	2.4537	1.946	20.7^{c}	52.86	17.62	11.927	Iguchi et al. (1984)
$WO_3 \cdot H_2O$	tungstite	Salmo, British Columbia, Canada	2.09	2.24	2.26	2.1967	1.820	17.1^{c}	72.15	18.03	13.838	Hellwege and Hellwege (1962)
$WO_2(OH)_2$	tungstite	Wolframocker, Salmo, British Columbia, Canada	2.09	2.24	2.26	2.1967	1.820	17.1^{c}	72.15	18.03	13.838	Larsen (1921)
$WO_3 \cdot 0.5H_2O$	hydrokenoelsmoreite	Elsmore, New South Wales, Australia	2.24	2.24	2.24	2.24	1.826	18.5^{c}	66.38	18.97	13.127	Williams et al. (2005)

$CaZr_{0.91}Ti_{0.06}Hf_{0.03}BAl_9O_{18}$	painite	Mogok Township, Pyin-Oo-Lwin district, Mandalay division, Myanmar	1.8159	1.8159	1.7875	1.8064	1.799	0.4	278.6	15.48	37.274	Shigley et al. (1986)
$Ca_4Al_2SO_4(OH)_{12} \cdot 6H_2O$	kuzelite	Zeilberg Quarry, Maroldsweisach, Franconia, Bavaria, Germany	1.504	1.504	1.488	1.4987	1.499	-0.1	256.5	23.31	21.35	Lerch et al. (1929)
ThO_2		Synthetic	2.105	2.105	2.105	2.105	2.078	1.3	43.9	21.95	7.851	Ellis and Lindstrom (1964)
LiOH		Synthetic	1.4639	1.4639	1.4518	1.4599	1.458	0.1	27.44	27.44	2.105	Shannon et al. (2002)
$LiAl_2(OH)_7 \cdot 2H_2O$		Synthetic	1.545	1.545	1.555	1.5483	1.547	0.1	169.81	18.86	15.548	Thiel et al. (1993)
$NaSb(OH)_6$	mopungite	Mopung Hills, Nevada	1.614	1.614	1.605	1.611	1.635	-1.5	125.55	20.92	12.804	Williams (1985)
$Be(OH)_2$	clinobehoite	Murzinkha region, Ural Mts., Russia	1.539	1.544	1.548	1.5437	1.536	0.5	37.22	18.61	3.379	Voloshin et al. (1991)
$Mg(OH)_2$	brucite	Wood Mine, Lancaster, Pennsylvania	1.5665	1.5665	1.5853	1.5728	1.565	0.5	40.9	20.45	3.911	Shannon et al. (2002)
$Mg_{0.94}Mn_{0.126}Sn_{0.97}(OH)_6$	schoen-fliesite	Pitkaranta, Republic of Karelia, Russia	1.667	1.667	1.667	1.667	1.660	0.4	117.73	19.62	13.091	Nefedov et al. (1977)
$Ca(OH)_2$	portlandite	Scawt Hill, Antrim County, Northern Ireland	1.575	1.575	1.547	1.5657	1.558	0.5	54.78	27.39	5.174	Tilley (1933)
$Ca_{0.98}Mg_{0.02}Sn(OH)_6$	burtite	El Hamman, Morocco	1.633	1.633	1.633	1.633	1.644	-0.6	134.15	22.35	14.168	Sonnet (1981)
$Ca_3Al_2(OH)_{12}$	katoite	Synthetic	1.605	1.605	1.605	1.605	1.599	0.3	247.97	20.66	25.042	Flint et al. (1941)
$Ca_3Fe_2(OH)_{12}$	hydro-	Synthetic	1.724	1.724	1.724	1.724	1.735	-0.6	260	21.67	31.323	McConnell

	andradite											(1964)
$Mn(OH)_2$	pyrochroite	Langban, Sweden	1.723	1.723	1.681	1.709	1.706	0.2	45.24	22.62	5.34	Palache et al. (1944)
$Mn_{0.95}Mg_{0.03}Ca_{0.02}Sn(OH)_6$	wickmanite		1.705	1.705	1.705	1.705	1.701	0.3	122	20.33	14.322	Moore and Smith (1968)
$Fe_{1.05}Mn_{0.01}Ge_{0.95}(OH)_6$	stottite	Tsumeb, Namibia	1.738	1.738	1.731	1.7357	1.731	0.2	106.5	17.75	13.031	Strunz et al. (1958)
$FeSn(OH)_6$	natanite		1.755	1.755	1.755	1.755	1.766	-0.6	113.69	18.95	14.264	Marshukova et al. (1982)
$Ni(OH)_2$	theophrastite	Vermion, Greece	1.759	1.759	1.759	1.759	1.750	0.5	39.28	19.64	4.954	Marcopoulos and Economou (1981)
$Zn(OH)_2$	ashoverite	Ashover, Derbyshire, England	1.629	1.629	1.639	1.6323	1.616	1.0	48.56	24.28	5.123	Clark et al. (1988)
$Zn(OH)_2$	sweetite	Derbyshire, England	1.635	1.635	1.628	1.6327	1.617	1.0	48.47	24.24	5.116	Clark et al. (1984)
$AlO(OH)$	bohmite	Ratnapura gem gravel, Sri Lanka	1.648	1.657	1.668	1.6577	1.661	-0.2	32.32	16.16	3.544	Sahama et al. (1973)
$Al_{0.99}Fe^{3+}_{0.01}(OH)_3$	gibbsite	Chester or Richmond, Massachusetts	1.568	1.568	1.587	1.5743	1.571	0.2	53.06	17.68	5.088	Larsen (1921)
$CrO(OH)$	grimaldiite	Merume River, Guyana	2.155	2.155	1.975	2.095	2.107	-0.7	34.25	17.12	6.076	Milton et al. (1976)
$Mn^{3+}O(OH)$	manganite	Thuringia, Germany	2.26	2.26	2.54	2.3533	2.321	1.4	33.27	16.64	7.082	Larsen (1921)
$Fe^{3+}O(OH)$	goethite	Restormel Royal Iron Mines, Lanlivery, Cornwall, England, UK	2.275	2.409	2.415	2.3663	2.267	4.2[b]	34.65	17.33	7.434	Bailly (1948)
$Fe^{3+}O(OH)$	goethite	Negaunee, Michigan	2.26	2.39	2.4	2.35	2.267	3.5[b]	34.65	17.33	7.361	Posjnak and Merwin (1919)
$Fe^{3+}O(OH)$	lepidocrocite	Easton Pennsylvania	1.938	2.2	2.515	2.2177	2.169	2.2	37.34	18.67	7.27	Posjnak and Merwin (1919)
$In_{0.86}Fe_{0.14}(OH)_3$	dzhalindite	Synthetic	1.725	1.725	1.725	1.725	1.720	0.3	62.8	20.93	7.576	Genkin and Muraveva

										(1964)
La$(OH)_3$	1.74	1.74	1.768	1.7493	1.753	-0.2	71.53	23.84	8.91	Roy and McKinstry (1953)

Notes: a = sterically strained compounds with strong bond-valence deviations; b = compounds with edge- and face-sharing MO_6 octahedra (M = Fe^{3+}, Mn^{3+}, Ti^{4+}, V^{5+}, Mo^{6+} and W^{6+}; c = compounds with corner-sharing octahedral; d = oxide ion conductivity

Table 3. Chemical compositions from chemical analyses and the corresponding normalized composition for 6 silicates, 5 phosphates, 1 arsenate and 2 sulfate minerals.

Mineral and location	Not normalized	Normalized	Reference
SILICATES			
ferronordite-La Lovozero massif, Russia	$(Na_{2.92}Ca_{0.08})(Sr_{0.99}Ba_{0.02})_{\Sigma 1.01}(La_{0.57}Ce_{0.41}Pr_{0.05}Nd_{0.04})_{\Sigma 1.07}Fe_{0.43}Mn_{0.29}Zn_{0.23}Mg_{0.06}(Si_{5.92}Al_{0.02})_{\Sigma 5.94}O_{17}$	$(Na_{2.92}Ca_{0.08})(Sr_{0.99}Ba_{0.01})_{\Sigma 1.0}(La_{0.53}Ce_{0.38}Pr_{0.05}Nd_{0.04})_{\Sigma 1.0}(Fe_{0.43}Mn_{0.29}Zn_{0.23}Mg_{0.06})(Si_{5.92}Al_{0.08})_{\Sigma 6.0}O_{17}$	Pekov et al. (2002)
scandio-babingtonite Montecatini Granite Quarry, Baveno, Novara, Italy	$(Ca_{1.71}Na_{0.25})_{\Sigma 1.96}(Fe_{0.65}Mn_{0.32})_{\Sigma 0.97}(Sc_{0.91}Sn_{0.04}Fe^{3+}_{0.03})_{\Sigma 0.98}Si_5O_{14}(OH)$	$(Ca_{1.74}Na_{0.26})_{\Sigma 2.0}(Fe_{0.67}Mn_{0.33})_{\Sigma 1.0}(Sc_{0.93}Sn_{0.04}Fe^{3+}_{0.03})_{\Sigma 1.0}Si_5O_{14}(OH)$	Orlandi et al. (1998)
marianoite Prairie Lake, Ontario, Canada	$(Ca_{4.0}Mn_{0.04})_{\Sigma 4.04}(Na_{1.93})(Nb_{0.97}Zr_{0.90}Ti_{0.09}Fe_{0.08}Mg_{0.03})_{\Sigma 2.07}Si_4O_{16.93}F_{1.07}$	$(Ca_{3.96}Mn_{0.04})_{\Sigma 4.0}(Na_{1.93})(Nb_{0.93}Zr_{0.86}Ti_{0.09}Fe_{0.08}Mg_{0.03})_{\Sigma 1.99}Si_4O_{16.93}F_{1.07}$	Chakhmouradian et al. (2008)
krauskopfite Rush Creek area, Mono County, California	$(Ba_{1.03}K_{0.01}Ca_{0.01})_{\Sigma 1.05}Si_{1.95}O_{4.95} . 3.08H_2O$	$(Ba_{0.98}Ca_{0.02})_{\Sigma 1.0}Si_2O_5 . 3H_2O$	Alfors et al. (1965)
okhotskite Kokuriki mine,Hokkaido, Japan	$(Ca_{1.91}Na_{0.04})_{\Sigma 1.95}(Mn_{0.69}Mg_{0.28})_{\Sigma 0.97}(Mn^{3+}_{1.13}Al_{0.47}Fe^{3+}_{0.40}Ti_{0.005})Si_{3.03}O_{9.93}(OH)_{4.07}$	$(Ca_{1.95}Na_{0.05})_{\Sigma 2.0}(Mn_{0.71}Mg_{0.29})_{\Sigma 1.0}(Mn^{3+}_{1.13}Al_{0.47}Fe^{3+}_{0.40}Ti_{0.005})Si_3O_{9.93}(OH)_{4.07}$	Togari and Akasaka (1987)
magnesio-neptunite Upper Chegem caldera near Mt.Lakargi,No. Caucasus, Russia	$(K_{0.67}Na_{0.32}Ca_{0.016})(Na_{2.06})(Li)(Mg_{1.39}Fe_{0.71})\Sigma 2.1(Ti_{2.03})_{\Sigma 2.03}(Si_{7.9}Al_{0.02})_{\Sigma 7.92}O_{24}$	$(K_{0.67}Na_{0.32}Ca_{0.016})(Na_2)(Li)(Mg_{1.32}Fe_{0.67})_{\Sigma 1.99}(Ti_2)_{\Sigma 2.0}(Si_{7.99}Al_{0.01})_{\Sigma 8.0}O_{24}$	Zadov et al. (2011)
PHOSPHATES			
natrophilite Brancheville, Conn.	$(Na_{0.93}Li_{0.02})_{\Sigma 0.95}Mn_{0.93}Fe_{0.07}PO_{3.95}(OH)_{0.05}$	$(Na_{0.96}Li_{0.04})_{\Sigma 1.0}Mn_{0.93}Fe_{0.07}PO_{3.95}(OH)_{0.05}$	Moore(1972)
maricite Big Fish River area, Yukon Territory, Canada	$(Na_{0.91})_{\Sigma 0.91}(Fe_{0.89}Mn_{0.07}Mg_{0.03})_{\Sigma 0.99}P_{1.02}O_4$	$(Na)_{\Sigma 1.0}(Fe_{0.90}Mn_{0.07}Mg_{0.03})_{\Sigma 1.0}PO_4$	Sturman et al. (1977)
nacaphite Mt. Rasvumchorr, Khibina massif, Russia	$Na_{1.99}(Ca_{0.94}Sr_{0.01}Mn_{0.01})_{\Sigma 0.96}PO_{3.97}F_{0.97}$	$Na_2(Ca_{0.96}Sr_{0.02}Mn_{0.02})_{\Sigma 1.0}PO_4F$	Khomyakov et al. (1981)
woodhouseite White Mountains, CA	$(Ca_{0.73}Sr_{0.04}Ba_{0.17}Na_{0.01})_{\Sigma 0.95}Al_{2.99}[P_{01.06}S_{0.97}O_4](OH)_6$	$(Ca_{0.76}Sr_{0.04}Ba_{0.19}Na_{0.01})_{\Sigma 1.0}Al_{2.99}[P_{01.06}S_{0.97}O_4](OH)_6$	Wise (1975)
birchite Broken Hill, New So. Wales, Australia	$(Cu_{1.94}Zn_{0.10})_{\Sigma 2.04}(Cd_{2.09}Ca_{0.02}Mn_{0.02})_{\Sigma 2.13}P_{2.07}S_{0.88}O_{12} . 5H_2O$	$(Cu_{1.90}Zn_{0.10})_{\Sigma 2.0}(Cd_{1.96}Ca_{0.02}Mn_{0.02})_{\Sigma 2.0}P_{2.07}S_{0.88}O_{12} . 5H_2O$	Elliott (2008)

ARSENATES			
cobalt-korignite Saxony Erzgebirge Germany	$(Co_{0.68}Zn_{0.24}Cu_{0.02}Fe_{0.01}Ni_{0.01})_{\Sigma 0.96}AsO_3OH \cdot H_2O$	$(Co_{0.71}Zn_{0.25}Cu_{0.02}Fe_{0.01}Ni_{0.01})_{\Sigma 1.0}AsO_3OH \cdot H_2O$	Schmetzer et al. (1981)
SULFATES			
leightonite Chuquicamata, Chile	$(K_{1.92}Na_{0.12})_{\Sigma 2.04}Ca_2Cu[SO_4]_4 \cdot 2H_2O$	$(K_{1.92}Na_{0.08})_{\Sigma 2.0}Ca_2Cu[SO_4]_4 \cdot 2H_2O$	Palache (1938)
kamchatkite Tolbachik volcano, Russia	$K(Cu_{2.92}Zn_{0.04})_{\Sigma 2.96}(SO_4)_2O_{1.04}Cl_{0.84}$	$K(Cu_{2.92}Zn_{0.08})_{\Sigma 3.0}(SO_4)_2OCl$	Vergasova et al. (1990)

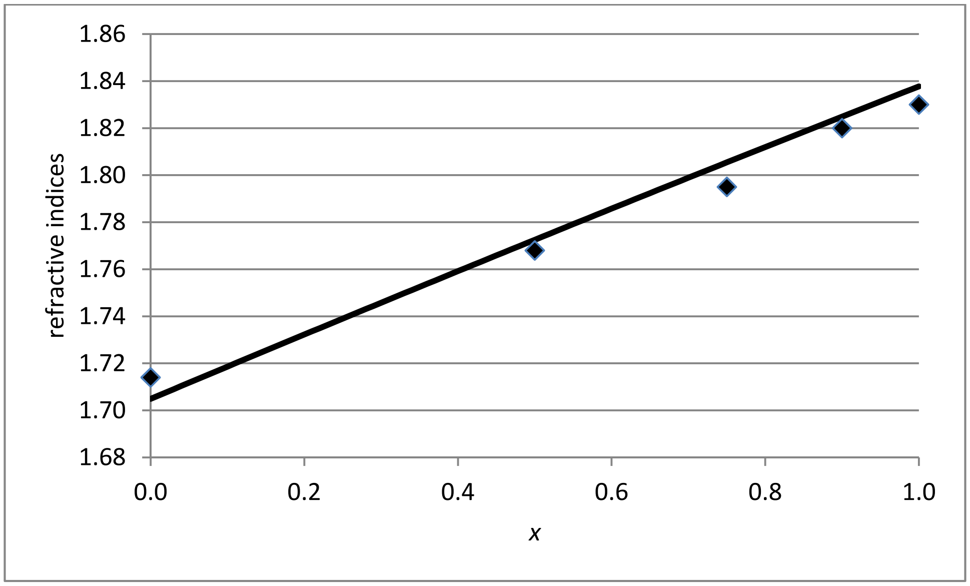

Figure 1. Refractive indices of pyrope-knorringite solid solutions $Mg_3(Al_{1-x}Cr_x)_2Si_3O_{12}$. Lattice parameter of knorringite from Novak and Gibbs (1971), *a* = 11.64 Å (α(Al) = 0.47 Å^3, α(Cr) = 3.02 Å^3), the line is calculated from polarizabilities, points are from Ringwood (1977).

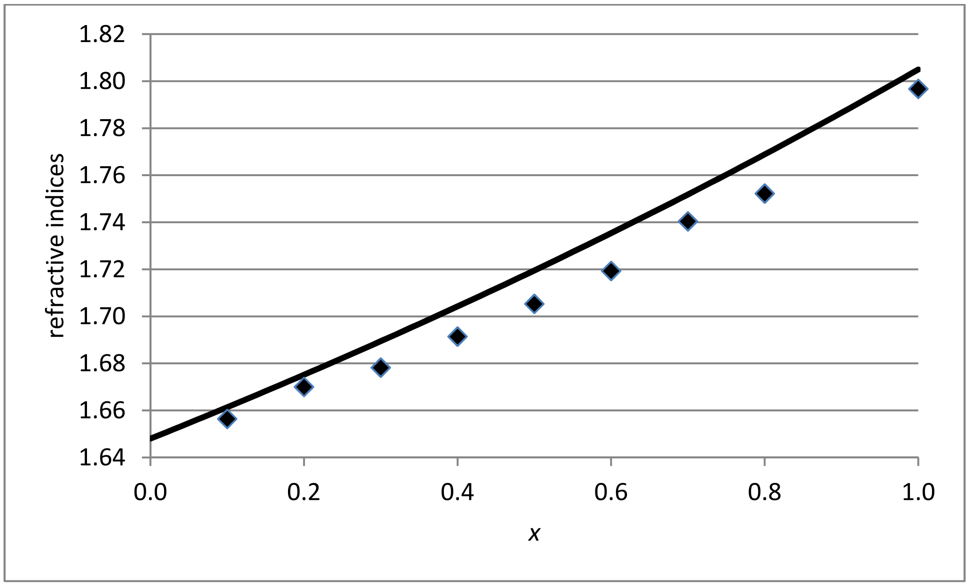

Figure 2. Refractive indices of tephroite-γ- Ca_2SiO_4 series $(Mn_xCa_{1-x})_2SiO_4$ (Greer, 1932) (α(Ca) = 1.79 $Å^3$, α(Mn) = 2.07 $Å^3$).

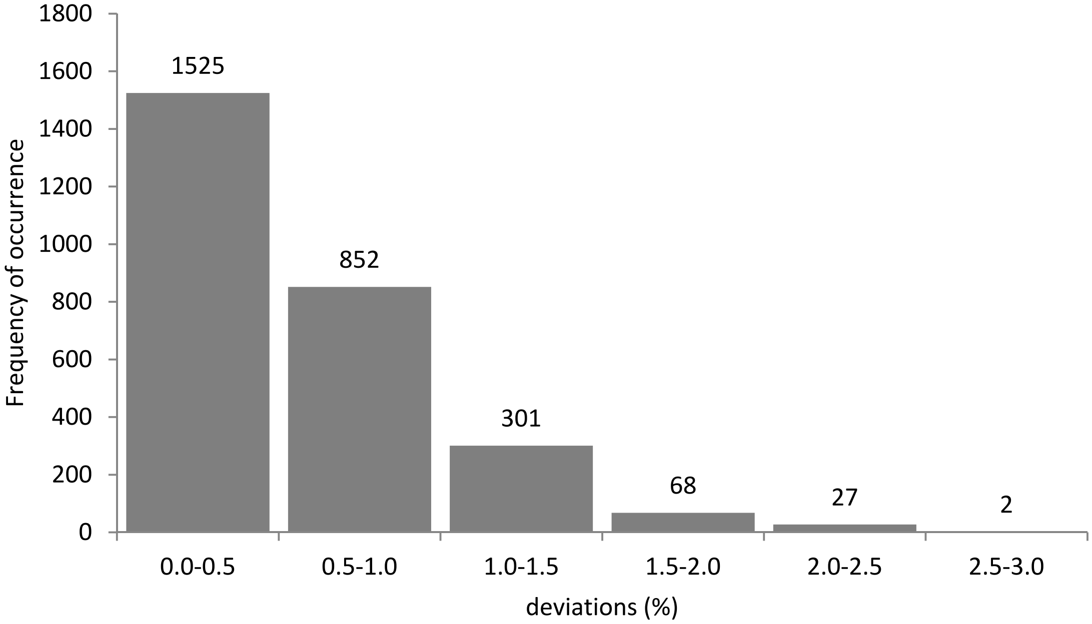

Figure 3. Frequency of occurrence of absolute values of deviations between observed and calculated refractive indices $\left|\frac{n_{obs}-n_{calc}}{n_{obs}}\right| \cdot 100$ in Table S1 (supplementary data[1]) in the range from 0 % to 3 %, excluding entries with systematic deviations as indicated in the remarks column of Table S1.