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 (2016) to determine the polarizabilities of 270 cations and anions removing 425 minerals and compounds containing the lone-pair ions (Ti4+, Sn5+, Pb2+, As3+, Sb5+, Bi3+, S4+, Se4+, Te6+, Cl−, Br−, I−) and uranyl ions, UO22+. 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 nD, nE, nP, <nDcalc>, (all determined at 589.3 nm), <nDcalc>, deviation of observed and calculated mean refractive indices, molar volume Vm, corresponding to the volume of one formula unit, anion molar volume Vam calculated from Vm divided by the number of anions (O2−, F−, Cl−, OH−) and H2O in the formula unit, the total polarizability <αAE>, and finally the reference to the refractive indices for all 2946 entries. The total polarizability of a mineral, <αAE>, is a useful property that reflects its composition, crystal structure, and chemistry and was calculated using the Anderson-Eggleton relationship

\[
\alpha_{AE} = \frac{\left(nD^2 - 1\right)V_m}{4\pi + \left(\frac{4\pi}{3} - c\right)\left(nD^2 - 1\right)}
\]

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, <αAE>, derived from individual polarizabilities of cations and anions. The deviation between observed and calculated refractive indices is <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 Ln3+ 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.