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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 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, $\langle n_{Dobs} \rangle$ (all determined at 589.3 nm), $\langle n_{Dcalc} \rangle$, 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 $\langle \alpha_{AE} \rangle$, and finally the reference to the refractive indices for all 2946 entries. The total polarizability of a mineral, $\langle \alpha_{AE} \rangle$, is a useful property that reflects its composition, crystal structure, and chemistry and was calculated using the Anderson-Eggleton relationship

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

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, $\langle \alpha_{AE} \rangle$ 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