American Mineralogist, Volume 103, pages 1345–1348, 2018

LETTER

POLARIO, a computer program for calculating refractive indices from chemical compositions

REINHARD X. FISCHER[1,*], MANFRED BURIANEK[1], AND ROBERT D. SHANNON[2]

[1]Universität Bremen, FB 5 Geowissenschaften, Klagenfurter Str. 2, D-28359 Bremen, Germany
[2]Geological Sciences/CIRES, University of Colorado, Boulder, Colorado 80309, U.S.A.

ABSTRACT

POLARIO is a computer program to calculate total electronic polarizabilities, refractive energies, and refractive indices of transparent minerals and synthetic crystalline compounds from their chemical composition and molar volume. If measured refractive indices or observed polarizabilities are entered, POLARIO also allows calculation of the deviation between observed and calculated values and determines the compatibility index as a measure of agreement. The density of the compound is calculated from the chemical composition and the molar volume of a formula unit. Atom parameters can be read in cif format to determine possible coordination numbers of cations and to compose the entire input necessary to do the calculations. It displays a table of interatomic distances and angles, and it shows the chemical composition with superscripted coordination numbers and valencies. The program is written in Delphi XE6 for WINDOWS operating systems and contains 5300 constants and parameters to do the calculations.

Keywords: Refractive index, total electronic polarizabilities, refractive-index calculation, Anderson-Eggleton relationship, Gladstone-Dale relationship, computer program