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A Windows program for chlorite calculation and classification

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ABSTRACT

A Microsoft Visual Basic program, WinCcac, has been developed to calculate the structural formulae of chlorite. WinCcac classifies rock-forming chlorite group minerals based on 14 oxygens for complete chlorite analyses. For electron-microprobe-derived chlorite analyses site occupancy can be estimated by using the stoichiometric H₂O (wt%) and Fe₂O₃ (wt%) contents. The program is created to predict cation site-allocations at the different structural positions such as the tetrahedral, octahedral, and interlayer sites. Furthermore, various chlorite geothermometers based on an empirical approach are carried out to specify the condition of formation temperature. WinCcac allows the user to enter and load multiple chlorite analyses in its own data entry window, to edit and load Microsoft Excel files in estimating and classifying chlorite data, and to generate and store all the calculated results in the output of Microsoft Excel file for further data evaluation and graphing purposes.

Keywords: Chlorite; Classification; Geothermometer; Software

1. Introduction

Chlorite is a common rock-forming mineral that formed in a variety of rocks and geological environments including sedimentary, low-grade metamorphic and hydrothermally altered rocks (De Caritat et al., 1993; Vidal et al., 2001; Deer et al., 2009). Chlorite group minerals are hydrous phyllosilicates with structures based on regularly alternating tetrahedral-octahedral 2:1 layers and interlayer octahedral cations (Krivovichev et al., 2004).

A general crystallochemical formula of chlorite based on 14 oxygens can be written to be :

$(R_x^{2+} R_y^{3+} \square_{6-x-y})_6^{VI} (Si_z R_{4-z}^{3+})_4^{IV} O_{10} (OH)_8$, where $R_x^{2+} = Fe^{2+}, Mg^{2+}, Mn^{2+}, Ni^{2+}, Co^{2+}, Zn^{2+}$, and

Cu^{2+} ; $R_y^{3+} = Al^{3+}, Fe^{3+}, \pm Cr^{3+}, \pm V^{3+}$; \square = octahedral vacancy; $R_z^{3+} = Al^{3+}, \pm B^{3+}, \pm Fe^{3+}$ (after

Zane and Weiss, 1998). Although not represented in this general crystallochemical formula,

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† The program is available from the journal server or from corresponding author on request

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