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Identification of Some Zeolite Group Minerals by Application of Artificial Neural Network and Decision Tree Algorithm Based on SEM-EDS Data

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Identification of zeolite group minerals is complicated due to their similar chemical formulas and habits. Although the morphologies of various zeolite crystals can be recognized under Scanning Electron Microscope (SEM), it is relatively more challenging and problematic process to identify zeolites using their mineral chemical data. SEMs integrated with energy dispersive X-ray spectrometers (EDS) provide fast and reliable chemical data of minerals. However, considering elemental similarities of characteristic chemical formulae of zeolite species (e.g. Clinoptilolite ($(Na,K,Ca)_{2-3}Al_3(Al,Si)_2Si_{13}O_{36}12H_2O$) and Erionite ($(Na_2,K_2,Ca)_2Al_4Si_{14}O_{36}\cdot 15H_2O$)) EDS data alone does not seem to be sufficient for correct identification. Furthermore, the physical properties of the specimen (e.g. roughness, electrical conductivity) and the applied analytical conditions (e.g. accelerating voltage, beam current, spot size) of the SEM-EDS should be uniform in order to obtain reliable elemental results of minerals having high alkali (Na, K) and H_2O (approx. %14-18) contents.

This study which was funded by The Scientific and Technological Research Council of Turkey (TUBITAK Project No: 113Y439), aims to construct a database as large as possible for various zeolite minerals and to develop a general prediction model for the identification of zeolite minerals using SEM-EDS data. For this purpose, an artificial neural network and rule based decision tree algorithm were employed. Throughout the analyses, a total of 1850 chemical data were collected from four distinct zeolite species, (Clinoptilolite-Heulandite, Erionite, Analcime and Mordenite) observed in various rocks (e.g. coals, pyroclastics). In order to obtain a representative training data set for each minerals, a selection procedure for reference mineral analyses was applied. During the selection procedure, SEM based crystal morphology data, XRD spectra and re-calculated cationic distribution, obtained by EDS have been used for the characterization of the training set. Consequently, for each zeolite species 250 EDS data (as elemental intensities) used for training and 200 $\pm$50 analyses were tested. Finally, two prediction models were developed. The constructed models with various cross-correlation values (r) yielded an average accuracy of $>$91% for the best predictions using C5.0 Decision Tree algorithm and back propagation artificial neural network. Despite having similar accuracies, the developed models exhibit different prediction behaviors for some zeolite minerals. The results demonstrate that artificial neural network as a nonlinear tool and decision tree algorithm as a rule based prediction model would be employed to provide considerably efficient and reliable identification/classification of some zeolite minerals regardless of their similar elemental compositions.

Keywords: mineral identification; zeolites; energy dispersive spectrometry; artificial neural networks; decision tree.