Tracking of hydration states of sulfates by laboratory and *in situ* Raman spectroscopy

FILIP KOŠEK[1] *, ADAM CULKA[1] AND JAN JEHLIČKA[1]

[1] Institute of Geochemistry, Mineralogy and Mineral Resources, Faculty of Science, Charles University, Prague, 128 43, Czech Republic (*correspondence: filip.kosek@natur.cuni.cz)

Polyhydrated sulfates are widespread secondary minerals on Earth. Furthermore, sulfate deposits have been detected in many Martian regions [1], and there are speculations about the presence of certain sulfates on the icy surface of moon Europa [2]. Polyhydrated sulfates also play an important role as indicators of past and present geochemical conditions. A fast and reliable analytical method for the investigation of their hydration state is required.

Water molecules incorporated into the crystal structure of sulfates affect the arrangement of coordination polyhedrons and change the length of S-O bonds. Raman spectroscopy is sensitive to this change resulting in a small shift of sulfate Raman bands according to actual hydration states within sulfate group of the same chemism [3].

Results of the laboratory analysis include Raman spectroscopic description of well-defined synthetic and natural polyhydrated sulfate phases (generally Fe-, Al-, and Mg-containing ones). Obtained data are valuable for the identification process of minerals in the areas such as volcanic vents or planetary surfaces. Presented data successfully show advantage in using of miniature hand-held Raman instruments and Raman microspectrometers for the characterization of sulfates from real geological settings [4].

The current study is focused on the of uncommon occurrence of sulfates on a burning coal dump Heřmanice, Ostrava, Czech Republic. This site provides a unique opportunity to study changes in hydration states of sulfates. Due to exceptional temperature and chemical conditions, anhydrous sulfates such as efremovite, godovikovite, sabieite or pyracmonite can coexist here with hydrated phases, e.g tschermigite, in a close proximity. Obtained results show, that anhydrous and hydrated sulfates are very well distinguishable by hand-held Raman spectrometers. Therefore, even a water content can be estimated according to the specific positions of sulfate bands in the *in situ* Raman spectra.

[1] Carter et al. (2012) *J. Geophys. Re. – Planet* 118, 831; [2] Shirley et al. (2010) *Icarus* 210, 358; [3] Wang and Zhou (2014) *Icarus* 234, 162; [4] Košek et al. (2017) *J. Raman Spectrosc.* (in press)