STATE OF WATER MOLECULES AND SILANOL GROUPS IN OPAL MINERALS: A NEAR INFRARED SPECTROSCOPIC STUDY OF OPALS FROM SLOVAKIA

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Recently near infrared spectroscopy in combination with double derivative technique has been effectively used by Christy [1] to differentiate between free silanol groups and hydrogen bonded silanol groups on silica gel. The method has given some insight into the type of functionalities and their location in silica gel samples. The inportant information in this respect comes from the overtones of the OH groups of water molecules hydrogen bonded to free silanol groups, and hydrogen bonded silanol groups absorbing in the region 5500-5100 cm^{-1} region. The approach was adapted to study the state of water and silanol functionalities and their locations in opals from Slovakia.

Twenty opal samples classified into CT and A classes and one quartz sample were used in this work. The samples were crushed using a hydrolic press and powderised. Each sample was then subjected to evacuation process to remove surface adsorbed water at 200 °C and the near infrared spectrum of the sample was measured using a Perkin Elmer NTS near infrared spectrometer equipped with a transflectance accessory. The detailed analysis of the sample was carried out using the second derivative profile of the spectrum. The samples were also heated to 750 °C to study the state of water molecules in Opal minerals.

The results indicate that the opal samples contain 1) surface adsorbed water 2) free and hydrogen bonded silanol groups on the surface 3) Trapped water in the bulk 4) free and hydrogen bonded silanol groups in the cavity surfaces in the bulk. A part of the water molecules found in the bulk of opal minerals are free molecules and the rest are found in hydrogen bonded state to free and hydrogen bonded silanol groups.

[1] A. A. Christy, New insights into the surface functionalities and adsorption evolution of water molecules on silica gel surface: A study by second derivative Near Infrared Spectroscopy, Vib. Spectrosc. 54 (2010) 42-49.