Spectroscopic characterization of brazilian emeralds from Tocantins State: Preliminary results

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Brazil is a major producer of emeralds, with many occurrences located in the southeastern, central and northeastern part of the country. In general, each emerald occurrence around the world has a specific spectroscopic, isotopic and geochemical signature, which can be important diagnoses as to the origin of this gemstone. About sixty emerald samples from Tocantins State, Brazil, were analyzed by essentially spectroscopic methods: Raman spectroscopy and molecular absorption spectroscopy in the ultraviolet-visible and near infrared (UV-Vis-NIR) region, besides single crystal x-ray diffraction, in order to obtain a characterization of fluid components (H_2O types I II and III, CO_2, CH_4) present in the crystalline structure of the mineral, defining the chromophore elements / causes of color, as well as the presence and nature of "impurities" in the form of alkaline elements present in the structural channels. Data were provided for the determination of emerald polytypes according to the position of the elements in the crystalline structure and their respective replacements, classifying the analysed samples as type-O. The presence of the fluid components H_2O types I, II and CO_2 was evidenced, as well as data for determination of the chromophore elements as Cr, V and Fe, their ionic charge and position into the crystalline structure. The effects of IVCT and LMCT were also demonstrated.