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Determination of the molar absorption coefficient for the infrared absorption band of CO_2 in rhyolitic glasses

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ABSTRACT

A new calibration was performed for the molecular CO_2 band at 2349 cm^{-1} in the infrared absorption spectra of rhyolitic glasses. Glasses with varying amounts of CO_2 (730–3900 ppm by weight) and H_2O (0.5–7.0 wt%) were synthesized in an internally heated pressure vessel at 200–800 MPa and 1100 and 1200 °C. The CO_2 content of the glasses was measured by coulometric CO_2-titration after thermal extraction at 1200 °C. It is shown that the entire CO_2 content cannot be extracted from a rhyolitic glass at this temperature. Using the Lambert-Beer law, and taking into account the residual CO_2 still present in the glasses after extraction, we have calculated a linear molar absorption coefficient of 1214 ± 78 $L \cdot cm^{-1}/mol$ for the band at 2349 cm^{-1}. Strictly, this value is a practical absorption coefficient because the IR band intensity is related to the total CO_2 content and not to the molecular CO_2 content. However, no direct evidence for other carbon species such as carbonate groups is found in the IR spectra. Hence, we suggest that the concentration of carbonate in the studied metaluminous rhyolite is negligible and the derived value is close to the real absorption coefficient for molecular CO_2. The absorption coefficient does not vary noticeably with changing water content of the glasses. With the new calibration, CO_2 concentrations in rhyolitic glasses are 13% higher than data based on the previous calibration of Blank (1993) for water-poor glasses.