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Determination of pressure in aqueo-carbonic fluid inclusions at high temperatures from measured Raman frequency shifts of CO_2

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Abstract

Due to the presence of additional volatiles and/or electrolytes in CO_2-H_2O fluids, the total pressure of many natural aqueo-carbonic fluid inclusions at high temperatures as determined using microthermometry is usually made with considerable uncertainty. In this paper, we present the results of our high *P*-*T* in situ Raman scattering study of high-density aqueo-carbonic fluids, with and without a small amount of CH_4 and NaCl, whose objective is to derive a new method for pressure determination in aqueo-carbonic fluid inclusions at high temperatures. The measurement of the Fermi dyad bands at temperatures up to 400 °C and pressures up to 1200 MPa is described. The manner in which the frequency shifts and intensity of Raman bands are governed by pressure, temperature, presence of CH_4 in carbonic and NaCl in aqueous fluids is discussed. From the monotonic dependence of the frequency shifts of the lower Fermi dyad band v_- and the Fermi resonant splitting D ($D = v_+ - v_-$) with pressure and temperature, the pressure (in MPa) in aqueo-carbonic fluid inclusions at elevated temperatures can be determined directly by using the following two polynomial equations:

$$P\,(\text{MPa}) = -16 + 1.232\times T - 53.72\times(\Delta v_-) - 1.83\times 10^{-3}\times T^2 + 24.46\times(\Delta v_-)^2 - 0.292\times T\times(\Delta v_-),$$
$$P\,(\text{MPa}) = -26 + 1.501\times T + 193.24\times(\Delta D) - 1.61\times 10^{-3}\times T^2 + 5.436\times(\Delta D)^2 + 0.158\times T\times(\Delta D),$$

where T is in °C, Δv_- and ΔD represent frequency shifts (in cm^{-1}) of the lower band and the resonant splitting relative to the reference values measured at 23 °C and 6 MPa, respectively. Based on the attainable accuracy of the fitted peak positions and the results from fitting of Raman frequency shifts' dependence with pressure and temperature, the uncertainty in pressure determination is about 50 MPa for pressures determined from v_- and 40 MPa from that determined from D.

Keywords: CO_2, Raman spectroscopy, pressure determination, HDAC, fluid inclusion