Estimation of pH in quartz-hosted fluid inclusions by coupling Pitzer-Duan thermodynamic modeling, Raman spectroscopy, LA-ICPMS analysis and microthermometric data.

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pH plays a key role in mineral solubility hence, the determination of pH is an important parameter to understand metal transport properties in paleofluids. Here we present a software program developed to determine the pH of paleofluids trapped in fluid inclusions. pH estimation of paleofluids can be obtained using fluid-mineral equilibria, however, in this study, our approach is on the H_2O–CO_2–Na-K-Ca-Mg-Cl–HCO_3^- system, more specifically by focusing on the CO_2/HCO_3^- equilibrium that occurs at the trapping temperature of paleofluids in fluid inclusions. First, the HCO_3^--CO_3^{2-}-CO_2 concentrations in the aqueous phase are obtained by Raman analysis at room temperature. Then the cations/Na ratios are measured using LA-ICPMS. The CO_2 and HCO_3^- concentrations and microthermometric data of ice melting temperature associated with a Pitzer thermodynamic model of this phase transition allows for the calculation of the concentration of the different aqueous species [1]. In the following step, we determine the CO_2 density in the vapor phase. This is accomplished by using the concentration of aqueous CO_2 and all other cations and anions combined with a dissymmetric thermodynamic model of CO_2 solubility at room temperature [2]. The concentration of the total carbon species measured by Raman spectroscopy at the homogenization temperature combined with the Duan model allows for the calculation of the bulk ϱ-x properties [3]. Finally, the pH is calculated along the isochores by using a combination of the models of Duan [3] and HKF [4]. The program can be applied for pressures and temperatures below 2000 bar and 523 K, respectively and NaCl concentrations below 5 molal.

[1] Pitzer et al. (1973) *J. Phys. Chem.* **77**, 268–277. [2] Duan et al. (2003) *Geochim. Cosmochim. Acta* **72** 5128-5145 [3] Duan et al. (2008*) Geochim. Cosmochim. Acta* **67** 671-680 [4]Sverjensky et al. (1997) *Geochim. Cosmochim. Acta* **61** 1359-1412.