Raman spectroscopic study of fluids containing H_2S in the fused silica capillary high-pressure optical cell

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Hydrogen sulfide (H_2S) is widely found in the atmosphere, natural gas, and fluid inclusions in minerals, and is an important component of mid-ocean-ridge hydrothermal fluxes. It also provides the required anions for the precipitation of transition metals from hydrothermal fluids. Therefore, it played an important role in the formation of volcanogenic massive sulfide ore deposits and orogenic gold deposits, and was involved in many other geological processes. Knowing the basic physicochemical properties of H_2S and other related geological fluids will enhance our ability for understanding or formulating models of geological processes.

Fused silica capillary can be used to construct ideal containers for the study of H_2S, because unlike precious metal containers (e.g., Au, Ag), it is inert to H_2S, and transparent to light of various wavelengths, making it suitable for in situ observation and sample characterization with spectroscopic methods. In this study, pure H_2S was sealed in a fused silica capillary capsule using the method of Chou et al. [1]. In combination with Linkam CAP500 heating-cooling stage [2], we performed a total of 82 measurements on the positions of the H_2S Raman ν_1 band between 188.15 and 372.15 K, and pressures (P) below 8.9 MPa in the co-existing liquid (L) and vapor (V) phases of H_2S with densities between 0.0005 and 0.9916 g/cm^3. The relation among H_2S density (ρ in g/cm^3), H_2S ν_1 peak position (in cm^{-1}), and temperature (T, in K) can be represented by: $\rho\ (\pm 0.0073) = -\ 958.68483 + 0.062922 \times T + 0.7579473 \times \nu_1 - 3.0174393 \times 10^{-7} \times T^2 - 2.379793 \times 10^{-6} \times T \times \nu_1 - 1.4966321 \times 10^{-4} \times \nu_1^2$ (with $r^2 = 0.9998$). This equation can be applied to calculate the density of the H_2S fluid from the measured H_2S ν_1 peak position at a given temperature. Our results are in good agreement with the sparse data collected in a limited T range between 282 and 373.4 K, and mostly along the L-V coexisting P-T curve [3]. Our Raman spectroscopic study of H_2S will soon be extended to the systems containing additional H_2O, CO_2, and metal(s) components at various P-T conditions.

[1] Chou et al. (2008) *Geochim. Cosmochim. Acta*, **72**, 5217-5231. [2] Chou (2012) *EMU Notes in Mineral.*, **12**, 227-247. [3] Salmoun et al. (1994) *J.* Raman. *Spectrosc.,* **25**, 281-287.