

Determination of NaCl-H₂O Isochores Using α - β Quartz Transition Pressure Calibrant and Quartz Raman Shift-Based Pressure Sensor in Hydrothermal Diamond-anvil Cell Experiments

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Existing NaCl-H₂O isochores, primarily derived from the synthetic fluid inclusion (SFI) method, exhibit limited precision, particularly when extrapolated beyond 600 MPa. This limitation arises because SFIs do not maintain strict isochoric conditions during heating under 1 atm external pressure. In this study, we employed a hydrothermal diamond-anvil cell (HDAC) to determine NaCl-H₂O isochores using two independent methods: (1) the α - β quartz transition pressure calibrant and (2) a pressure sensor based on the Raman shift of the quartz 128 cm⁻¹ band (ω_{128}). Prior to each isochore determination, the HDAC sample chamber was conditioned through multiple heating-cooling cycles to ensure isochoric behavior. The salinity of the sample solutions was calculated from the measured ice melting temperature after completing a series of isochore determinations. Based on 53 measurements of solutions with NaCl concentrations ranging from 5.7 to 21.2 wt%, the refined isochores can be expressed by:

$$P(\text{bar}) = A_1 + A_2 \times T(^{\circ}\text{C}) \quad (1)$$

where A_1 and A_2 are functions of NaCl molality and the vapor-to-liquid homogenization temperature (T_h). These isochores are valid up to ~1.2 GPa and ~900 °C. Fig. 1 compares two representative isochores derived from Eq. (1) with those obtained using the SFI method [2].

Additionally, the isochores were independently determined using a newly established pressure-sensor equation for quartz [3] in HDAC experiments. The pressures on the isochores were calculated from measured temperatures and ω_{128} values (large dots in Fig. 1). The close agreement between the isochores derived from Eq. (1) and those obtained using the quartz pressure sensor confirms the reliability of both methods for isochore determination.

Figure 1. NaCl-H₂O isochores calculated from Eq. (1) for two solutions with specified T_h (solid lines), compared with those from [2] (dashed lines with dotted extensions above 600 MPa). The P - T points (large dots) are derived from the pressure sensor equation [3].

References

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