

Molar absorptivities of OH and H₂O in rhyolitic glass at room temperature and at 400–600 °C

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ABSTRACT

We determined near-infrared (NIR) molar absorptivities of hydroxyl group (4500 cm⁻¹) and molecular water (5230 cm⁻¹) in rhyolitic glasses at room temperature and at high temperature, 400–600 °C. Five rhyolitic glasses with 0.5–2.8 wt% total water were analyzed by FT-IR microspectroscopy at room temperature and at 50 °C intervals in the range of 400 to 600 °C using a heating stage. The total water contents in the rhyolitic glasses were measured by Karl-Fischer titration. Based on these data, the linear molar absorptivities of the 4500 and 5230 cm⁻¹ bands at room temperature were determined to be 1.42 ± 0.12 and 1.75 ± 0.08 L/mol-cm, respectively. The integral molar absorptivities obtained are 285 ± 24 and 239 ± 11 L/mol-cm² for the 4500 and 5230 cm⁻¹ bands, respectively. These values can be used to determine the concentrations of hydroxyl group and molecular water in rhyolitic glass with 0.5–2.8 wt% total water at room temperature. The experimental results at high temperature show that the linear and integral molar absorptivities of the 4500 cm⁻¹ band at 400–600 °C generally remain within 6% of the values at room temperature. On the other hand, the linear and integral molar absorptivities of the 5230 cm⁻¹ band systematically decrease with increasing temperature in the ranges of 400 to 600 °C. These high-temperature molar absorptivities are useful for evaluating the water speciation in rhyolitic glass by in situ high-temperature IR microspectroscopy.