Densities of dilute coenzyme M solutions to 0.80 MPa and 353.15 K

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Sodium 2-mercaptoethanesulfonate (C₅H₇NaO₃S₂), also known as coenzyme M is a thiol that is essential to the process of methanogenesis [1]. Coenzyme M is a cofactor involved in methyl transfer reactions within methanogenic archaea. Given that fossil evidence of methanogenic archaea may date back to 2.8 billion years [2], methanogenesis is likely an ancient metabolic process. Determining the thermodynamic properties of coenzyme M is essential for understanding the potential for its formation and reaction properties in high P-T environments that host extremophiles and may have hosted the emergence of life.

The volumetric properties of dilute aqueous solutions of coenzyme M (0.09966 m, 0.19950 m, 0.299921 m & 0.39815 m) were obtained using an Anton Paar DMA 5000 vibrating tube densimeter. Reproducibility of density measurements was <±0.00002 g·cm⁻³, exceeding propagated errors associated with uncertainty in the measurement of temperature, pressure, and fluid concentration.

Experimentally determined volumetric properties of coenzyme M have not been previously reported in the literature. Figure 1 shows partial molar volumes at infinite dilution (V∞) derived from fluid density data; it is clear that V∞ is not a sensitive function of pressure in the range examined.

![Graph](image)

**Figure 1.** Experimentally determined partial molar volumes at infinite dilution of sodium 2-mercaptoethanesulfonate in aqueous solutions at 0.10-0.80 MPa and 293.15-353.15 K from this study. Lines represent simple linear regression fits to the data. The error bar represents the estimated uncertainty of ±1.0 cm³·mol⁻¹.