Experimental Study of Triflic Acid and Sodium Triflate in Aqueous Solutions: Standard Molar Volumes and Heat Capacities up to 573 K and 28 MPa

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For predicting the solubility, reactivity, and transport of radionucleides in geological fluids, their thermodynamic properties at high temperatures are needed. In this connection, it is of interest to obtain data on trivalent lanthanide cations, since they are fission products and analogues of actinides that are difficult to study directly. In order to avoid the complexing of these highly charged cations, it is convenient to study them in combination with the bulky monovalent thifluoromethanesulphonate (triflate) anions, which are known as poor ligands and are remarkably stable at high temperatures. For extracting the thermodynamic properties of lanthanide cations, it is necessary to first have reliable data on the contribution of the triflate anion. Such data are, however, only limited. The main purpose of this study is to extend the knowledge of the standard derivative properties of the triflate anion over a wide range of temperatures and pressures.

We have obtained the densities and specific heat capacities of aqueous solutions of triflic acid (HCF_3SO_3) and sodium triflate (CF_3SO_3Na) at temperatures up to 300 °C and at pressures to 28 MPa. The measurements were performed for dilute solutions (0.025 to 0.4 molal) with a flow vibrating tube densimeter [1] and a high temperature Picker calorimeter [2] constructed in the Laboratory. The standard molar volumes and heat capacities of the solutes were obtained via the apparent molar properties extrapolated to infinite dilution with use of the Pitzer ionic interaction model. Using the standard molar volumes and heat capacities of NaCl(aq) and HCl(aq) from literature, it was possible to calculate the specific contribution of the triflate ion. Our results are compared with earlier investigations [3-4].

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