Isobaric Heat Capacity of Water

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Abstract

Water is an anomalous and unique liquid in the sense that some of its physical properties do not exhibit monotonous behaviour when plotted against temperature. For example, isobaric heat capacity exhibits a minimum near 37 C. No theory/model is available in the literature to explain this behaviour of isobaric heat capacity with temperature. We, therefore, suggest a model to study the isobaric heat capacity of water as a function of temperature. The model is based on two-state theory of water in which water is considered as a mixture of two species. One of the specie is called open-packed specie resembling with ice structure and having mole fraction as X0 whereas the other is called closed-packed species resembling with un-hydrogen bonded water molecules and having mole fraction as Xc=1- X0 .An empirical relation is developed as a function of temperature for open-packed specie using the data reported by Davis and Litovitz [J.Chem.Phys. 42,2563 (1965)]. On the basis of this mixture model, isobaric heat capacity of water is assumed as

$$Cp=X0\ Cp0+(1-X0\ )Cpc$$

Further Cp0 and Cpc are considered as a function of temperature. The computation of heat capacity indicates a minimum near 40 C which is in very good agreement with experimental results.