XXXV SALÃO de INICIAÇÃO CIENTÍFICA

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The water, besides being essential for human life, is largely used in several industrial processes, often mixed with other substances. Particularly, alcohols are used as cosolvents in aqueous systems. The water in itself presents more than 70 anomalies, among which specific heat, density and compressibility play important roles. For instance, at fixed pressure, the density of pure water changes with temperature, having a maximum at 4°C. In a mixture with a small amount of tert-butanol, the temperature of maximum density and the specific heat increases, suggesting the occurrence of water aggregation promoted by the alcohol. In this work we check this hypothesis of water aggregation by the alcohol both by experiments and simulations, for different temperatures and alcohol concentrations. We use Small-Angle X-ray Scattering (SAXS) and Molecular Dynamics Simulations. From the experimental data we show that small aggregates are formed, whose radius of gyration increases with alcohol concentration, reaches a maximum, and decreases for further alcohol addition. We also show that the scattering intensity at zero angle, which is related to the isothermal compressibility, follows the same behavior of the radius of gyration. From the computational data we extract the change in temperature of maximum density which also increases with the addition of alcohol. Our results support the hypothesis that a small amount of alcohol favors the formation of aggregates.

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