



Contribution ID: 430

Type: **Poster**

Aqueous solutions of heterocyclic amines: structure and thermodynamics

Monday 20 March 2023 16:00 (2 hours)

Heterocyclic amines, such as piperidine and N-methylpiperidine aggregate in aqueous solutions due to hydrogen bonds between hydration water molecules. No such aggregation occurs in the mixtures of these amines with other hydrogen-bonded solvents, such as methanol or ethanol. This difference highlights the active role of water solvent in promoting the self-aggregation. However, the role of various contributions in thermodynamic functions due to specific interactions, van der Waals forces, and the effect of the size and shape of the molecules remains open. In the present communication we explore and discuss the family of solutions of pyrrolidine, piperidine, and their methylated counterparts in water and in methanol, as revealed by thermodynamic measurements as well as by direct visualization of the mesoscopic structure employing small-angle neutron scattering. While the limiting partial molar enthalpies of solutions of pyrrolidine, N-methylpyrrolidine, piperidine, and N-methylpiperidine in methanol follow closely the trend assessed from theoretically calculated molecular interaction energies, their behavior is markedly different in water solutions, and can be described by taking into account an empirical hydrophobic hydration term.

Small angle neutron scattering evidenced that the aqueous amine solutions are microheterogeneous on the nanometer-order length scale. Various models are considered to describe the structural arrangement of the hydrated amine molecules. The tendency of approaching phase separation increases in the order: N-methylpiperidine < N-methylpyrrolidine < piperidine < pyrrolidine.

Authors: ALMÁSY, László (Centre for Energy Research); FEHÉR, Bence (Eindhoven University of Technology); AVDEEV, Mikhail (Joint Institute for Nuclear Research); MARCZAK, Wojciech (Jan Długosz University in Czestochowa)

Presenter: ALMÁSY, László (Centre for Energy Research)

Session Classification: Poster Session MONDAY

Track Classification: Glasses and Liquids