

## عنوان مقاله:

On the properties of N-methyl- $\gamma$ -pyrrolidonium hydrogen sulfate ionic liquid and alkanol mixtures

## محل انتشار:

هفتمین کنفرانس ملی نوآوری و فناوری علوم زیستی و شیمی ایران (سال: 1402)

تعداد صفحات اصل مقاله: 6

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## خلاصه مقاله:

The properties of N-methyl- $\gamma$ -pyrrolidonium hydrogen sulfate mixed with alkanols are studied as a function of mixtures composition and temperature. Experimental physicochemical properties combined with molecular simulation (quantum chemistry and classical molecular dynamics) were considered, thus providing a micro and macroscopic characterization of fluids' structuring, intermolecular forces and molecular aggregation. The results were analyzed in thermodynamics terms considering deviations of ideality and mixing properties as well as from the coordination and interaction between the involved ions and molecules by the developed complex hydrogen bonding networks. The results allow a multiscale characterization of the considered mixed systems thus providing the required information for the possible applications of low viscous protic pyrrolidonium based ionic liquids and their mixtures with relevant hydrogen bonding molecular cosolvents.

## کلمات کلیدی:

.Ionic liquids, Mixtures, Pyrrolidone, Sulfate, Thermodynamics, Molecular dynamics

## لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/1766999>

