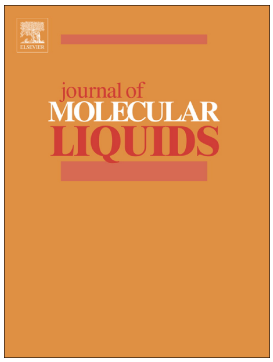

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Physicochemical properties of alkanolamine-choline chloride deep eutectic solvents: Measurements, group contribution and artificial intelligence prediction techniques

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ABSTRACT

Further development in the utilization of deep eutectic solvents (DESs) for new processes requires an insightful understanding of their fundamental properties. Hence, in this study, we report experimental measurements of the density, viscosity, conductivity, pH, surface tension and thermal stability of three different amine based deep eutectic solvents (DESs), (Choline chloride + monoethanolamine, ChCl-MEA), (Choline chloride + diethanolamine, ChCl-DEA) and (Choline chloride + methyldiethanolamine, ChCl-MDEA), representing the primary, secondary and tertiary amines, respectively. The experimental data was obtained at temperature from 293.15-353.15 K and for three different choline chloride to amine molar ratios of 1:6, 1:8 and 1:10. Moreover, the densities of the amine based DESs were predicted with the empirical group contribution method, conventional artificial neural network (ANN) and bagging artificial neural network (ANN). Due to the special nature of bonds that exists between the alkanol-amines and the choline chloride salt, the deviations for the traditional group contribution and ANN methods are quite high when compared to the experimental values. Hence, a technique based on bagging ANN, which combines the results of several ANNs in order to reduce the deviations and errors, was established. The experimental results revealed that amine-based DESs are more thermally stable as compared to stand-alone amine solvents. The density, viscosity, stability and conductivity increased with decreasing choline chloride to amine molar ratio in the DESs. However, there was no clear trend in the pH with molar ratio. The bagging ANN provided the best prediction for both the density and