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## The effect of temperature on cation aggregation in dodecyl betaine Nacyl glycinate amino acid ionic liquid: Molecular dynamics simulation investigation

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The effect of temperature on the cation aggregation in dodecyl betaine N-acyl glycinate amino acid ionic liquid (AAIL) surfactant was studied using molecular dynamics (MD) simulation. The structure of the AAIL is shown in Figure 1.



Fig. 1 Schematics of a) N-acyl glycinate anion and b) dodecyl betaine cation

Radial distribution function (RDF) for cation-cation, cation-anion, and anion-anion, mean square displacement (MSD) for cation, anion and water, root mean square displacement (RMSD) for micelle and root mean square fluctuation (RMSF) for cation and anion at three temperatures (290, 300 and, 310 K) were applied to obtain the results. RDF plots were almost the same because of similar interactions. The MSD decreases with temperature for cation, anion, and water since the mobility increases with increasing temperature. In addition, anion-water, cation-water, cation-anion, and anion-anion interactions become weak with temperature enhancement. RMSD plots for micelle at 290 and 300 K were almost the same though a significant increase is observed at 310 K indicating the micelles are less stable at 310 K according to Jana et al. results [1]. Moreover, RMSF of both cation and anion increased considerably at 310 K that confirmed the less rigidity at the highest studied temperature [2]. Based on the results, micelle stability is dependent on the temperature and the structural properties confirm the variation of the anion and cation positions.

## References

- [1] S. Jana, S. Dalapati, Sh. Ghosh, N. Guchhait, J Photochem Photobiol B. 2012, 112, 48.
- [2] A. Verma, A. Kumar, M. Debnath, Medicinal Chemistry Research, 2016, 25, 1616.