ANION-DRIVEN DESIGN OF IMIDAZOLIUM-BASED IONIC LIQUIDS: INTEGRATING PHYSICOCHEMICAL PROFILING, IONICITY ANALYSIS, DFT/ADMET MODELING AND ANTIMICROBIAL PERFORMANCE

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ABSTRACT

Ionic liquids represent a highly tunable class of compounds whose physicochemical and biological properties can be modified through rational selection of cations and anions. In this study, three imidazolium-based ionic liquids containing oxychlorine anions were synthesized and characterized: 1-butyl-3-methylimidazolium chlorite, chlorate and perchlorate. The main objective was to evaluate how progressive anion oxygenation affects density, viscosity, conductivity, ionicity and antimicrobial activity.

The synthesized ionic liquids were characterized by NMR and IR spectroscopy, while density, viscosity and electrical conductivity were measured from 293.15 to 323.15 K. Density decreased linearly with temperature, whereas viscosity decreased with increasing temperature. The perchlorate-based ionic liquid showed the highest density and viscosity, suggesting stronger structural organization and reduced expansivity. Conductivity measurements revealed the highest molar conductivity for the chlorate-based ionic liquid, indicating an optimal balance between ionicity and viscous resistance. Walden analysis showed that chlorate and perchlorate ionic liquids behaved close to the ideal KCl reference line, with ionicity values above 90%, while the chlorite-based ionic liquid exhibited lower ionicity and stronger ion association.

DFT calculations supported the experimental trends by revealing specific C–H···O interactions and differences in anion charge distribution. Antimicrobial activity was tested against *Escherichia coli*, *Staphylococcus aureus*, *Bacillus cereus* and *Candida guilliermondii*. The chlorite-based ionic liquid exhibited the strongest antimicrobial activity, likely due to enhanced formation of contact ion pairs or small aggregates that facilitate interactions with microbial cell envelopes.

Keywords: ionic liquids, oxychlorine anions, physicochemical properties, ionicity, antimicrobial activity, DFT calculations.

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