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Synthesis and thermal and structural characterization of novel Ionic Liquids with imidazolium cations and carboxylate anions.

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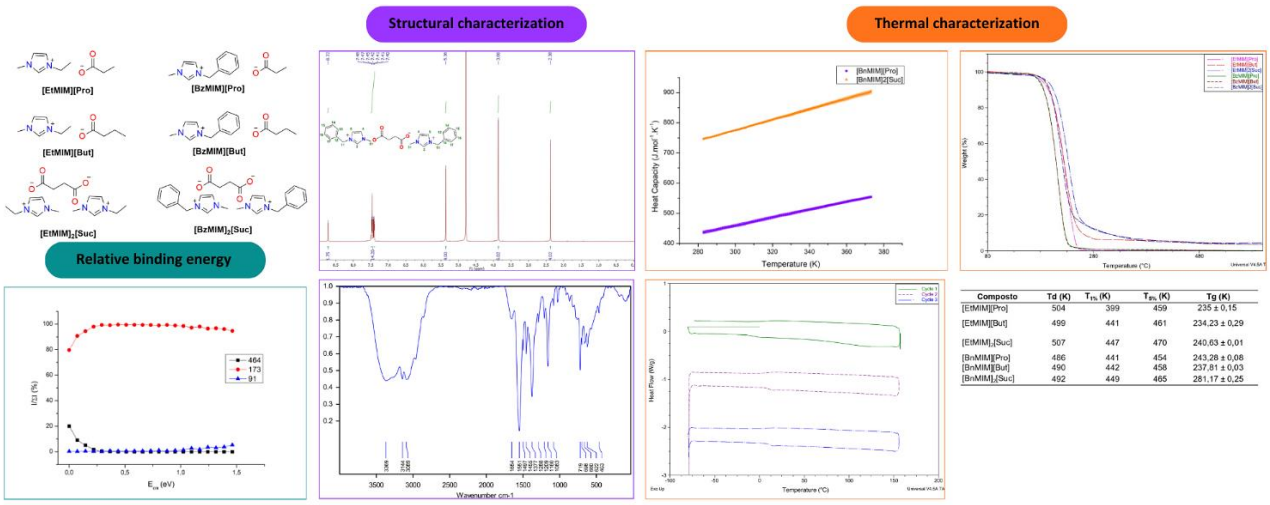
ABSTRACT

In this study, six ionic liquids (ILs), three of which are novel, were synthesized using ethyl-methyl-imidazolium or benzyl-methyl-imidazolium cations and carboxylate anions derived from propionic, butyric, succinic, and glutaric acids. The physicochemical properties of these compounds were evaluated and compared to determine the effects of structural modifications on the cations and anions. The synthesis involved an SN2 reaction of methylimidazole with the respective alkyl halide, followed by anion exchange (from halide to hydroxide) using an anion exchange resin and subsequent neutralization with acid. Structural characterization was conducted using NMR, ESI-MS-MS, and IR spectroscopy. Thermal properties were assessed through Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) to determine thermal stability and behavior, respectively. TGA revealed that structures with two carboxylates tend to decompose 5% and 10% at higher temperatures compared to analogous structures with a single carboxylate. No phase transitions were observed for any structures, indicating amorphous behavior within the studied temperature range (193 K to 433 K). Relative binding energy evaluation via ESI-MS-MS was assessed for $[BnMIM]_2[Suc]$. Specific heat capacity (Cp) measurements indicate that the presence of the second carboxylate group results in an increase in Cp compared to the analogous monocarboxylate, as expected due to the higher molecular mass of this structure. Additionally, qualitative and quantitative solubilities, bromide content, density, and the relative binding energies for the other compounds are being measured [1,2].



Composto	Td (K)	T_{m} (K)	T_{g} (K)	Tg (K)
[EtMIM][Pro]	504	399	459	235 ± 0,15
[EtMIM][But]	499	441	461	234,23 ± 0,29
$[EtMIM]_2[Suc]$	507	447	470	240,63 ± 0,01
[BnMIM][Pro]	486	441	454	243,28 ± 0,08
[BnMIM][But]	490	442	458	237,81 ± 0,03
$[BnMIM]_2[Suc]$	492	449	465	281,17 ± 0,25

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REFERENCES

(1) Freitas, A. M. S.; Vieira, J. C. B.; Beck, T. S.; Zibetti, L.; Villetti, M. A.; Frizzo, C. P.; Bender, C. R. Ionic Liquids Based on Carboxylate Anions: Auto and Hetero Assembly with Methylcellulose in Diluted and Semi-Diluted Regime. *Journal of Ionic Liquids* **2024**, *4* (1). https://doi.org/10.1016/j.jil.2024.100082.

(2) Frizzo, C. P.; Bender, C. R.; Salbego, P. R. S.; Farias, C. A. A.; Villetti, M. A.; Martins, M. A. P. Heteroassembly Ability of Dicationic Ionic Liquids and Neutral Active Pharmaceutical Ingredients. *ACS Omega* **2018**, *3* (2), 2282–2291. https://doi.org/10.1021/acsomega.7b02097.