Synthesis and Structural Characterization of 1-Butyl-2,3-dimethylimidazolium Bromide and Iodide

Johanna Kutuniva, Raija Oilunkaniemi, Risto S. Laitinen, Janne Asikkala, Johanna Kärkkäinen, and Marja K. Lajunen

Department of Chemistry, P.O. Box 3000, FI-90014 University of Oulu, Finland

Reprint requests to Prof. Risto Laitinen.
Fax: +358-8-553-1608. E-mail: risto.laitinen@oulu.fi

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1-Butyl-2,3-dimethylimidazolium bromide {(bdmim)Br} (**1**) and iodide {(bdmim)I} (**2**) were prepared conveniently by the reaction of 1,2-dimethylimidazole and the corresponding 1-halobutane. The compounds were characterized by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy as well as by X-ray single crystal crystallography. **1** crystallizes in the monoclinic crystal system, space group $P2_1/n$, with $Z = 4$, and unit cell dimensions $a = 8.588(2)$, $b = 11.789(1)$, $c = 10.737(2)$ Å, $\beta = 91.62(3)^\circ$. Compound **2** crystallizes in the monoclinic crystal system, space group $P2_1/c$, with $Z = 8$, and unit cell dimensions $a = 10.821(2)$, $b = 14.221(3)$, $c = 15.079(2)$ Å, $\beta = 90.01(3)^\circ$. The lattices of the salts are built up of 1-butyl-2,3-dimethylimidazolium cations and halide anions. The cations of **1** form a double layer with the imidazolium rings stacked together due to π interactions. The Br^- anions lie approximately in the plane of the imidazolium ring, and the closest interionic Br···H contacts span a range of 2.733(1) – 2.903(1) Å. Compound **2** shows no π stacking interactions. The closest interionic I···H contacts are 2.914(1) – 3.196(1) Å.

Key words: 1-Butyl-2,3-dimethylimidazolium Bromide, 1-Butyl-2,3-dimethylimidazolium Iodide, X-Ray Crystal Structure