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

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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 \(a = 8.588(2)\) Å, \(b = 11.789(1)\) Å, \(c = 10.737(2)\) Å, \(\beta = 91.62(3)\)°. Compound 2 crystallizes in the monoclinic crystal system, space group \(P2_1/c\), with \(Z = 8\), and unit cell dimensions \(a = 10.821(2)\) Å, \(b = 14.221(3)\) Å, \(c = 15.079(2)\) Å, \(\beta = 90.01(3)\)°. 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 \(\pi\) interactions. The \(\text{Br}^-\) anions lie approximately in the plane of the imidazolium ring, and the closest interionic \(\text{Br}^−\cdot\cdot\cdot\text{H}\) contacts span a range of 2.733(1) – 2.903(1) Å. Compound 2 shows no \(\pi\) stacking interactions. The closest interionic \(\text{I}^-\cdot\cdot\cdot\text{H}\) 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