Synthesis and Crystal Structures of 1-Alkoxy-3-alkylimidazolium Salts Including Ionic Liquids, 1-Alkylimidazole 3-oxides and 1-Alkylimidazole Perhydrates

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Functionalized quaternary imidazolium salts were prepared with the intention to obtain new ionic liquids (ILs). Thus, more than forty 3-alkoxy-1-alkylimidazolium salts, 3-alkoxy-1-alkyl-2-methylimidazolium salts, 1-methylimidazole 3-oxide and 1,2-dimethylimidazole 3-oxide as well as their salts, 1,3-dihydroxymimidazolium salts and 1,3-dihydroxy-2-methylimidazolium salts were synthesized and characterized by spectroscopy and, to a limited extent, by viscosity and conductivity measurements. Results of fourteen single crystal X-ray structure determinations are reported, among them also the parent compounds 1-hydroxymimidazolium 3-oxide and 1-hydroxy-2-methylimidazolium 3-oxide. Selective debenzylation of 1-benzyloxy-3-methyl imidazolium salts and mono-demethoxyla- tion of 1,3-dimethoxymimidazolium salts were achieved by hydrogenolysis. In addition, a crystalline semiperhydrate of 1,2-dimethylimidazole was characterized. Furthermore, an addition compound of 1-methylimidazole 3-oxide with tris(2-thienyl)borane and a silver carbene complex derived from 1-benzyloxy-3-methylimidazolium hexafluorophosphate was crystallized and characterized.

Key words: Carbene, Degradability, Imidazolium, Ionic Liquid, \textit{N}-Oxide, Perhydrate