Imidazolium Phenolates

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Dedicated to Professor Helmut Werner on the occasion of his 75th birthday

1,3-Diisopropyl-4,5-dimethylimidazolium phenolate (4a), pentafluorophenolate (4b), and pentachlorophenolate (4c) are obtained from 2,3-dihydro-1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene (2) and the corresponding phenols 3 as stable crystals in excellent yields. The crystal structure analyses of compounds 4 reveal the presence of ion pairs linked by almost linear C–H···O hydrogen bonds. With 4-hydroxypyridine (5), the carbene 2 gives 1,3-diisopropyl-4,5-dimethylimidazolium 4-pyridinolate (6) whose crystal structure analysis indicates the ions to be connected by a C–H···N bond.

Key words: Heterocycles, Imidazole, Phenol, Hydrogen Bond, Crystal Structure