Supramolecular Organization of Organoammonium Squarates

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Syntheses, thermal behavior, and IR data of three hydrogen squarates, Hsq^- , with 2-(acetyl-amino)-4-methylpyridinium, $[(C_8H_{11}N_2O)(HC_4O_4)]$ (1), 2-carboxamido-pyridinium, $[(C_6H_7N_2O)-(HC_4O_4)]$ (2), and 2-methylpyridinium cations, $[(C_6H_8N)(HC_4O_4)(H_2O)]$ (3), and one squarate, sq^{2-} , with 2-amino-4-methyl-pyrimidinium cations, $[(C_6H_9N_2)_2(C_4O_4)]$ (4) are reported. The crystal structures of 1 and 4 have been studied. The compounds decompose in two thermal stages: (i) release of organic base, (ii) decomposition of squarate. Crystallographic analyses show that 1 and 4 have S6, $R_2^2(10) R_2^2(9) R_2^2(7)$ rings. The hydrogen bonding motifs formed by the hydrogensquarate anions interact with the ammonium cations through N–H…O hydrogen bonds and give rise to predominantly layered structures, which also exhibit three-dimensional connectivity.

Key words: Squaric Acid, Organic Amine, Thermal Decomposition