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, [(C8H11N2O)(HC4O4)] (1), 2-carboxamido-pyridinium, [(C6H7N2O)-(HC4O4)] (2), and 2-methylpyridinium cations, [(C6H8N)(HC4O4)(H2O)] (3), and one squarate, sq2−, with 2-amino-4-methyl-pyrimidinium cations, [(C6H9N2)2(C4O4)] (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, R22(10) R22(9) R22(7) rings. The hydrogen bonding motifs formed by the hydrogen-squarate 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