Abstract

Combination of the compact but sterically flexible ferrocene scaffold with intermolecular binding potential and conformational variability of (2-hydroxyethyl)ammonium structural motif was utilised in the construction of solid crystalline materials. Crystallisation in systems containing ferrocenecarboxylic, 2-ferrocenylacetic, 3-ferrocenylpropionic, 3-ferrocenyl-acrylic, 3-ferrocenylacrylic, 3-ferrocenylpropiolic, ferrocene-1,1´-dicarboxylic or ferrocene-sulfonic acid with 2-aminoethanol afforded crystals of the corresponding salts. The resulting crystalline products were characterised with the usual methods (proton nuclear magnetic resonance, infrared spectroscopy, elemental analysis) and their crystal structures were determined by means of single-crystal X-ray diffraction analysis. The crystal structures of the salts mentioned above usually contain rather complicated two dimensional networks of charge-assisted hydrogen bonds. With the aim of studying potentially more simple hydrogen-bonded structures, additional crystallisation experiments were conducted in systems of ferrocenecarboxylic acid and 2-(methylamino)ethanol or 2-(dimethylamino)ethanol. These experiments yielded simple salt of the former amine and adducts of salts of both bases with ferrocenecarboxylic acid in the ratio of 1:1. The crystal structures of these compounds are based on layers similar to those observed in structures of salts of 2-aminoethanol. It has been observed, however, that some of these compounds readily undergo decomposition.

Keywords: crystal engineering, ferrocene, single-crystal X-ray diffraction analysis, infrared spectroscopy, (2-hydroxyethyl)ammonium salts, crystallization, crystal structure, charge-assisted hydrogen bonds, non-covalent interactions.