Intermolecular interactions of proton transfer compounds: synthesis, crystal structure and Hirshfeld surface analysis

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Description
Three new proton transfer compounds, [2-ammonio-5-methylcarboxybenzene perchlorate (1), (C8H10NO2+·ClO4−), 4-(ammoniomethyl)carboxybenzene nitrate (2), (C8H10NO2+·NO3−), and 4-(ammoniomethyl)carboxybenzene perchlorate (3), (C8H10NO2+·ClO4−)], have been synthesized, their IR modes of vibrations have been assigned and their crystal structures studied by means of single-crystal X-ray diffraction. Their asymmetric units consist of one cation and one anion for both compounds (1) and (2). However, the crystal structure of compound (3) is based on a pair of cations and a pair of anions in its asymmetric unit. The three-dimensional Hirshfeld surface analysis and the two-dimensional fingerprint maps revealed that the three structures are dominated by H···O/O···H and H···H contacts. The strongest hydrogen-bonding interactions are associated with O—H···O and N—H···O constituting the highest …