A Conformational Analysis of the Spirocyclic Quaternary Ammonium Cation $[(CH_2)_4N(CH_2)_4]^+$ in its Bromide and Picrate Salts

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High-yield syntheses of the bromide (1a) and picrate salts (1b) of the 5-azonia-spiro[4]nonane cation $[(CH_2)_4N(CH_2)_4]^+$ are reported. In the single crystal X-ray diffraction analyses of the two salts the spirocyclic quaternary ammonium cations have their five-membered rings in envelop and twist conformations modified by packing forces. The conformation found experimentally for 1a has C_2 -symmetry as predicted for the gas phase by quantum-chemical calculations (RI-DFT, RI-MP2), but the five-membered rings are intermediate between the expected envelop and the twist form. For 1b, both of the two independent cations can be described as a combination of rings in an envelop and a twist conformation. According to the NMR spectra, in solution the cations are highly flexible and pseudosymmetrical (point group D_{2d}).

Key words: Conformational Analysis, Spirocyclic Ammonium Salts, 5-Azoniaspirononane Cation, Heterospirononanes