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Synthesis, characterization and crystal structure of 9-aminoacridinum acridine-9-carboxylate proton transfer ion pair

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Abstract: 9-aminoacridinum acridine-9-carboxylate (1) as a proton transfer ion pair was obtained by the reaction of 9-aminoacridine, acridine-9-carboxylic acid and zinc nitrate (1:1:1 molar ratio) in solvents mixture H₂O/MeOH under reflux condition. The crystal structure of this compound was determined by elemental analysis, IR spectroscopy and single crystal X-ray diffraction method. Crystallographic data for 1 was collected at 100 K. The synthesized compound has been crystallized in monoclinic system with C2/c space group and a = 15.336 (9), b = 14.342(8), c = 19.481(1), $\beta = 109.057(1)$ cell parameters. The final R value is 0.044 for 4425 independent reflections. There are various types of ionic and non-covalent interactions including N–H…O hydrogen bonding, π - π stacking, and cationic-anionic interactions in the crystal structure of (1). This interactions play important role in the expansion of 3D network of (1).

Keywords: Acridine-9-carboxylic acid; ion pair; crystal structure; hydrogen bonding.

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