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Synthesis, Growth, Characterization and Quantum Chemical Investigations of an Organic Single Crystal: 2-Amino- 4-Methylpyridinium Quinoline- 2-Carboxylate

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Abstract : Interestingly, organic materials exhibit large optical nonlinearity with quick responses and having the flexibility of molecular tailoring using computational modelling and favourable synthetic methodologies. Pyridine based organic compounds and carboxylic acid contained aromatic compounds play a crucial role in crystal engineering of NCS complexes that displays admirable optical nonlinearity with fast response and favourable physicochemical properties such as low dielectric constant, wide optical transparency and large laser damage threshold value requires for optoelectronics device applications. Based on these facts, it was projected to form an acentric molecule of π-conjugated system interaction with appropriately replaced electron donor and acceptor groups for achieving higher SHG activity in which quinoline-2-carboyxlic acid is chosen as an electron acceptor and capable of acting as an acid as well as a base molecule, while 2-amino-4-methylpyridine is used as an electron donor and previously employed in numerous proton transfer complexes for synthesis of NLO materials for optoelectronic applications. 2-amino-4-mehtylpyridinium quinoline-2-carboxylate molecular complex (2AQ) is having π-donor-acceptor groups in which 2-amino-4-methylpyridine donates one of its electron to quinoline -2-carboxylic acid thereby forming a protonated 2-amino-4-methyl pyridinium moiety and mono ionized quinoline-2-carboxylate moiety which are connected via N-H…O intermolecular interactions with non-centrosymmetric crystal packing arrangement at microscopic scale is accountable to the enhancement of macroscopic second order NLO activity. The 2AQ crystal was successfully grown by a slow evaporation solution growth technique and its structure was determined in orthorhombic crystal system with acentric, P212121, space group. Hirshfeld surface analysis reveals that O…H intermolecular interactions primarily contributed with 31.0 % to the structural stabilization of 2AQ. The molecular structure of title compound has been confirmed by 1H and 13C NMR spectral studies. The vibrational modes of functional groups present in 2AQ have been assigned by using FTIR and FT-Raman spectroscopy. The grown 2AQ crystal exhibits high optical transparency with lower cut-off wavelength (275 nm) within the region of 275-1500 nm. The laser study confirmed that 2AQ exhibits high SHG efficiency of 12.6 times greater than that of KDP. TGA-DTA analysis revealed that 2AQ crystal had a thermal stability of 223 °C. The low dielectric constant and low dielectric loss at higher frequencies confirmed good crystalline nature with fewer defects of grown 2AQ crystal. The grown crystal exhibits soft material and positive photoconduction behaviour. Mulliken atomic distribution and FMOs analysis suggested that the strong intermolecular hydrogen bonding which lead to the enhancement of NLO activity. These properties suggest that 2AQ crystal is a suitable material for optoelectronic and laser frequency conversion applications.

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