A First Principles Study of Nonlinear Optical Properties of a Quinoline Derivative

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Abstract

A quinoline derivative, 4-(quinolin-2-ylmethylene)aminophenol was synthesized and structurally characterized by single crystal X-ray diffraction. The crystal packing behaviour and intermolecular interactions were examined by Hirshfeld surface analyses, 2D fingerprint plots and QTAIM analysis. The second order nonlinear response of 4-(quinolin-2-ylmethylene)aminophenol molecule immersed in DMSO was investigated at PCM/DFT/CAM-B3LYP/6-311++G(d,p) level. Theoretical calculations of the Hyper-Rayleigh scattering first hyperpolarizability were performed using two different procedures, the Sum-over-states scheme and the energy derivative method from Gaussian16. The HRS first hyperpolarizability results were compared with obtained for other organic compounds and shown that the 4-(quinolin-2-ylmethylene)aminophenol presents a good nonlinear optical response.

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