Structural, Electronic and Vibrational Properties of Chromene Derivative D

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Abstract:

Chromenes and their derivatives have been considered as an important class of oxygen-containing heterocycles. There has been an increasing interest in the study of chromenes due to their biological activity. Herein, the structural, electronic, and vibrational properties of a chromene derivative, entitled 2-amino-5-oxo-4-phenyl-4,5-dihydropyrano[3,2-c]chromene-3-carbonitrile and abbreviated as Chrom-D, have been reported. The FT-IR, UV-Vis. the molecular geometry is computed in the frame of density functional theory at the B3LYP/6-311++G(d,p) level of theory. the electronic properties of the title compound have been studied based on the TD-DFT . Finally, Chrom-D has been evaluated as a multifunctional agent against Alzheimer's disease (AD) .

Keywords: The FT-IR, UV-Vis, DFT, chromenes