CRYSTAL STRUCTURE OF N-(2,4-DIMETHOXYBENZYL)-2-(2-OXO-2H-CHROMEN-4-YLOXY)ACETAMIDE

Sharmila N1, T.V. Sunda2, M. Govindhan3, K. Subramanian4, V. Viswanathan5, D. Velmurugan5

1P.G And Research Department Of Physics, National College (Autonomous), Tiruchira, Tiruchirappalli-6, India, 2P.G And Research Department Of Physics, National College (Autonomous), Tiruchira, Tiruchirappalli-1, India, 3Department of Chemistry, Anna University, Chennai 600 025, India, 4Orchid Chemicals & Pharmaceuticals Ltd, R&D Centre, Sholinganallur, Chennai 600 119, India, 5Centre of Advanced Study in crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India

E-mail: 05.sharmi@gmail.com

Coumarin and its derivatives represent one of the most active classes of compound possessing a wide spectrum of biological activity. Its derivatives have been effectively used as anticoagulants for the treatment of disorders in which there is excessive or undesirable clotting, such as pulmonary embolism. The single crystal X-ray diffraction study of the title compound has been made and its structure is compared with the optimized structure obtained with MOPAC2016’s PM7 algorithm. The title compound, C20H19NO6, crystallized in the monoclinic space group P21. The unit cell parameters are a= 7.278 (5) Å, b= 8.576 (7) Å, c= 14.410 (12) Å with V= 897.4 (12) Å³ and Z=2. The dihedral angle between the 2H-chromen (C1-C9,O1) and the phenyl group (C13-C18) is 65.19 (19)°. The 2H-chromene ring system and the phenyl group is almost planar, with an r.m.s. deviations of the fitted atoms being 0.011 and 0.007Å. The structure was solved by direct methods using SHELXS-97 and refined by full matrix least square on F2 to an R-value of 0.08 for 1664 reflections (I>2σ(I)) using SHELXL-2014. The 2H-chromene ring system is puckered (puckering parameter Q= 0.018(9) Å) with the atom O1 showing the maximum deviation of 0.012(7) Å. The total energy and dipole moment of the title molecule are computed as -4668.59044 eV and 8.338 Debye respectively. A superimposed fit of the title compound and its energy minimized structure gives an r.m.s. deviation of 2.155Å. The crystal is stabilized by C—H•••O and N—H•••O intermolecular interactions. The interaction between C15 and O4 through H15 forms parallel chain motif C(8) along ‘c’ axis and the interaction between N1 and O4 through H1 forms parallel chain motif C(4) in a zig-zag manner along ‘b’ axis. These two interactions forms the three dimensionel framework.


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