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Vagish ChannaBasappa , Karthik Kumara , Lokanath K Neratur , Ajay Kumar Kariyappa

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Synthesis, crystal structure studies and Hirshfeld surface analysis of 6-chloro-7-hydroxy-4-methyl-2*H*-chromen-2-one

Vagish ChannaBasappa,[a] Karthik Kumara,[b] Lokanath K Neratur[b] and Ajay Kumar Kariyappa[a*]

[a]*Department of Chemistry, Yuvaraja's College, University of Mysore, Mysuru 570005, India.*
[b]*Department of Studies in Physics, Manasagangotri, University of Mysore, Mysuru 570006, India.*
Contact email: ajaykumar@ycm.uni-mysore.ac.in

Abstract: The title compound 6-chloro-7-hydroxy-4-methyl-2*H*-chromen-2-one, a coumarin derivative was synthesized and characterized by using spectroscopic tools such as mass spectra, NMR (^{1}H and ^{13}C) and finally the structure was confirmed by the single crystal X-ray diffraction studies. The title compound ($C_{10}H_7ClO_3$) crystallized in the monoclinic crystal system, with the space group $P2_1/n$. The cell parameters were confirmed by both powder and single crystal X-ray diffraction studies. The molecule is palnar with all the substituents at the same plane of the coumarin moiety. The crystal and molecular structure of the title compound is stabilized by inter molecular O—H···O and C—H···O hydrogen bonds. The structure also exhibits C—Cl···*Cg* halogen bond interactions and π···π stacking interactions, which contributes to the crystal packing. Further, Hirshfeld surface analysis was carried out to understand the intermolecular interactions along with their graphical visualization through 2D fingerprint plots.

Keywords: Crystal structure, X-ray diffraction, Hirshfeld surface analysis, Fingerprint plots, *Cg*···*Cg* interactions.

Specifications Table

Subject area	Chemical Physics
Compound	6-Chloro-7-hydroxy-4-methyl-2*H*-chromen-2-one
Data category	Synthesis, NMR (^{1}H and ^{13}C), mass spectra and crystallographic data.