



Synthesis, Spectral Study and Crystal Structure Analysis of Two Coumarin Derivatives

N. Latha Rani¹, Shivaprasad Shetty², N.V. Anil Kumar³ and M.A. Sridhar^{1*}

1. Department of Studies in Physics, Manasagangotri, University of Mysore 570 006, Mysuru, **INDIA**

2. Department of Chemistry, NMAM, Institute of Technology, Nitte, Karkala, Udupi, Karnataka, **INDIA**

3. Department of Chemistry, Manipal Institute of Technology, Manipal, Udupi, Karnataka, **INDIA**

Email: mas@physics.uni-mysore.ac.in

Accepted on 11th January 2018, Published online on 27th January 2018

ABSTRACT

In this paper we will discuss the crystal structure of two coumarin molecules Ethyl 2-(4-methyl-2-oxo-chromen-7-yl) oxyacetate (c4), 2-(4-Methyl-2-oxo-chromen-7-yl) oxyacetohydrazide (c5). The compound c4 crystallizes in the monoclinic crystal system with the space group $P2_1/n$. The unit cell parameters are $a = 12.502(3) \text{ \AA}$, $b = 8.324(2) \text{ \AA}$, $c = 13.477(3) \text{ \AA}$, $\beta = 115.558(15)$, $Z = 4$. The compound c5 crystallizes in the monoclinic crystal system with the space group $P2_1/c$. The unit cell parameters are $a = 10.0839(7) \text{ \AA}$, $b = 14.5972(12) \text{ \AA}$, $c = 8.4573(6) \text{ \AA}$, $\beta = 112.489(4)$, $Z = 4$.

Highlights

- Synthesis of two coumarin derivatives Ethyl 2-(4-methyl-2-oxo-chromen-7-yl) oxyacetate and 2-(4-Methyl-2-oxo-chromen-7-yl) oxyacetohydrazide has been discussed in this manuscript.
- The two coumarin derivatives were characterized by FTIR, ¹H NMR and single crystal X-ray diffraction.
- This manuscript highlights the details of structural study of two coumarin molecules.
- The two molecules crystallize in monoclinic crystal system.
- The molecular arrangement in the first compound shows that the formation of $R_2^2(22)$ through C-H...O hydrogen bonds.
- The second compound shows the formation of $R_2^2(6)$ inverted dimer through N-H...N hydrogen bonds and $R_2^2(12)$ inverted dimer through N-H...O hydrogen bonds.

Keywords: Coumarin, phytochemical, Graph-set theory, intermolecular interactions, intramolecular.