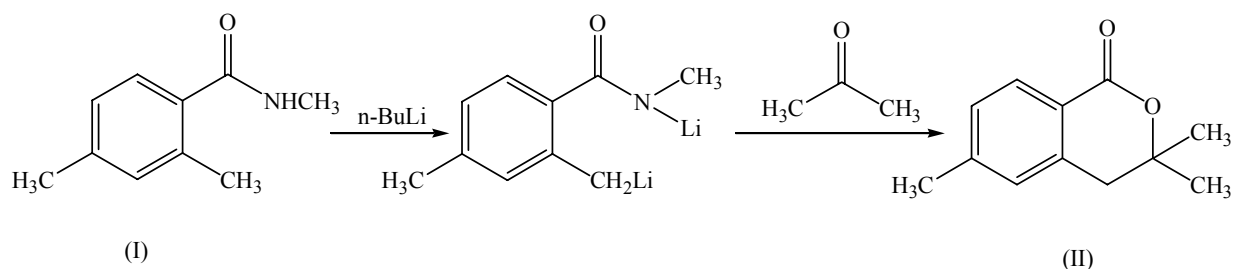


## X-ray crystallographic, spectroscopy and quantum chemical studies on 3, 3, 6-trimethyl-3, 4-dihydroiso-coumarin

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Structural and spectral characteristics of 3,3,6-trimethyl-3,4-dihydroiso-coumarin have been studied by methods of X-ray crystallography, infrared spectroscopy and quantum chemistry. The reaction mechanism of the compound crystallization is given below:



An irregular shaped crystal of dimensions 0.3 x 0.2 x 0.2 mm was selected for intensity data collection and the unit cell parameters were determined by least-squares fit of setting angles of 1880 reflections ( $\theta$  range 2.71-24.46°). The intensities were measured by the  $\phi$  and  $\omega$  scan method. The space group was determined to be  $P2_1/c$  from the systematic absences  $h0l: l = 2n + 1, 0k0: k = 2n + 1$ . Data were corrected for Lorentz-and polarization corrections. The structure was solved by direct methods using SHELXS86 software. The structure contains three crystallographically independent molecules, in the asymmetric unit. R-factor based on E-values,  $R_E = 0.217$ . The optimized geometry of the three molecules has been obtained by quantum chemical calculations by using DFT and RHF methods by using 6-311++G\*\* basis set. The optimized molecular geometries are in good agreement with the X-ray analysis. The geometry of all the three asymmetric molecules indicates similarity in terms of their bond distances and bond angles. However, pronounced differences are observed in the values of torsion angles. Based on the suitable scaled DFT/6-311G\*\* calculation, assignments have been provided to the fundamental vibrational bands of these molecules in terms of frequency, form and intensity of vibrations and potential energy distribution across the symmetry coordinates in the ground state.