

Ab Initio Calculations of pK_a Values for 7-Acetoxy coumarin-3-Carboxylic Acid

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In our study, *ab initio* calculations on 7-Acetoxy coumarin-3-Carboxylic Acid and its deprotonation mechanism was evaluated by theoretical calculations. The acidity constants, pK_a values have been determined by using B3LYP/6-31G(d) basis sets of density functional theory (DFT) along with physical and thermodynamic parameters. The geometries of all the structures have been fully optimized with the Gaussian-03 programme using the hybrid B3LYP method with a 6-31G* basis set. The *ab initio* geometries have been used in calculating the solvation free energies carried out using at he B3LYP/6-31G(d). The conversion factor of 1 Hartree = 627.5095 kcal mol⁻¹ was used since the total energies were given in Hartree.

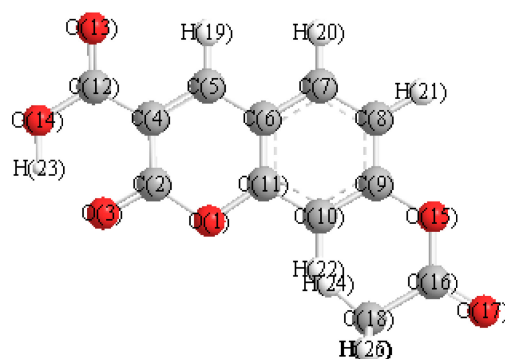


Fig. 1: The molecular structure of 7-Acetoxy coumarin-3-carboxylic acid.

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Acknowledgements

We are grateful to ESOGU for financial support through Research Project No: 200519010 and ESOGU Research Project No: 200819015.