CRYSTAL STRUCTURE OF (2R,3R)-ETHYL 2,3-DIMETHYL-4-OXO-6-PHENYL-3,4-DIHYDRO-2H-PYRAN-5-CARBOXYLATE

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4H-Pyran-4-ones and their various derivatives are known for their significance biological and pharmacological activities. They are shown to have a central depressant activity in mice, and ethylmaltol was found to be a potent anticonvulsant against convulsions induced by pentetrazole and strychnine. 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, C₁₆H₁₈O₄ is crystallized in the space group P₂₁/c. The 3,4-dihydro-2H-pyran-4-one moiety (C₇—C₁₁, O₁,O₂) forms a dihedral angle of 43.47 (9)° with the phenyl group. The unit cell parameters are a= 9.3042 (2) Å, b= 15.7535 (4) Å, c= 10.9923 (3) Å with V= 1509.32 (7) Å³ and Z=4. The structure was solved by direct methods using SHELXS-97 and refined by full matrix least square on F² to an R- value of 0.03 for 1438 reflections using SHELXL-2014. The pyran ring is puckered (puckering parameters: Q = 0.393 (4) Å, q₂ = 0.323 (4) Å, q₃ = 0.223 (4) Å, β =55.3 (6)° and φ = 273.8 (6)°, with atom C₈ deviating by -0.258 Å from the C₇/C₉–C₁₁/O₁ plane, the ring is in an envelope conformation. The HOMO and LUMO energy levels were found to be -9.719 and -0.898 eV, respectively. The total energy and dipole moment of the title molecule are computed as -3389.58771 eV and 5.546 Debye respectively. The relative conformation about the bond joining the 3,4-dihydro-2H-pyran-4-one moiety with the phenyl group is defined by the torsion angles C₁— C₆—C₇—O₁ and C₅— C₆—C₇—O₁ are [-43.1 (4)° and 135.2 (3)° in the crystal structure; -41.74° and 137.87° in the optimized structure] shows (-) syn-clinal and (+) Anti-clinal respectively. A superimposed fit of the title compound with its energy-minimized molecule gives an r.m.s. deviation of 3.668 Å. C—H•••π interactions were observed which stabilize the crystalline solid along the ab plane. Also weak π–π interactions contribute the three dimensional framework.

REFERENCES
Keywords: crystal structure, pyran-4-one, C—H•••π interactions