Poster Presentation

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Crystal Structures of Four Novel Thiophene/Phenyl-piperidine Hybrid Chalcones

M. Parvez[1], M. Bakhtiar[2], M. Baqir[3], M. Zia-ur-Rehman[2]

[1]University of Calgary, Department of Chemistry, Calgary, Canada, [2]University of the Punjab, Institute of Chemistry, Lahore, Pakistan, [3]PCSIR Laboratories, Lahore, Pakistan

Chalcones constitute an important class of bioactive drug targets in the pharmaceutical industry that includes anti-ulcerative drug sofalcone. In continuation of our work, the crystal structures of four closely related 1-phenyl-piperidine based chalcones will be presented. I: C19 H21NOS, MW = 311.43, T = 173(2) K, λ = 0.71073 Å, Orthorhombic, P b c a, a = 10.1045(4), b = 10.5358(4), c = 30.6337(12) Å, V = 3261.2(2) Å3, Z = 8, Dc = 1.269 Mg/m3, F (000) = 1328, R [I>2σ(I)] = 0.059. II: C18H19NOS, MW = 297.40, T = 173(2) K, λ = 1.54178 Å, Orthorhombic, P b c a, a = 8.9236(2), b = 11.0227(2), c = 30.8168(6) Å, V = 3031.21(11) Å3 Z = 8, Dc = 1.303 Mg/m3, F (000) = 1264, R [I>2σ(I)] = 0.035. III: C18H19NOS, MW = 297.40, T = 173(2) K, λ = 1.54178 Å, Orthorhombic, P b c a, a = 8.82990(10), b = 11.0061(2), c = 31.2106(5) Å, V = 3033.13(8) Å3, Z = 8, Dc = 1.303 Mg/m3, F (000) = 1264, R [I>2σ(I)] = 0.048. IV: C18H18ClNOS, MW = 331.84, T = 173(2) K, λ = 0.71073 Å, Monoclinic, P 21/c, a = 14.1037(4), b = 11.3153(3), c = 10.1290(2) Å, β = 101.1367(14)°, V = 1586.02(7) Å3, Z = 4, Dc = 1.390 Mg/m3, F (000) = 696, R [I>2σ(I)] = 0.038. The crystals of I, II and III are isomorphous. In all structures, the piperidine rings are in chair conformations, thiophene rings are essentially planar and the C=C bonds in the prop-2-en-1-one fragment adopt E-conformation. All crystal structures are devoid of any classical hydrogen bonds. However, non-classical hydrogen bonding interactions of the type C---H...O in compounds II, III and IV link the molecules into chains extended along the b-axis. Moreover, C---H...Cg interactions involving thiophene rings in I and III and benzene ring in IV and π…π interactions between benzene rings lying about inversion centers are present in II and III.

[1] *Hussain, T; Siddiqui, H. L; Zia-ur-Rehman, M; et al (SHELXL-97). Acta Cryst. 2008, A64, 112.*

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