

Single crystal X-ray studies and Hirshfeld surface analysis of ethoxy phenyl substituted chalcone derivatives

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S. Madan Kumar , K. Byrappa

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Chemical Data Collections article

Title: Single crystal X-ray studies and Hirshfeld surface analysis of ethoxy phenyl substituted chalcone derivatives

Authors: K. R. Harshitha^a, B. K. Sarojini^a, B. Narayana^b, Anupam. G. Lobo^c, S. Madan Kumar^d, K. Byrappa^e

Affiliations: ^aDepartment of Industrial Chemistry, Mangalore University, Mangalagangothri -574199, Mangaluru, Karnataka, India.

^bDepartment of Studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka, India

^cSchool of Chemical Sciences, Mahatma Gandhi University -686560, Kottayam, Kerala, India.

^dDST-PURSE Lab, Mangalore University, Mangalagangothri -574199, Mangaluru, Karnataka, India.

^eDepartment of Materials Science, Mangalore University, Mangalagangothri -574199, Mangaluru, Karnataka, India.

Contact email: bksaroj35@gmail.com

Abstract: The single crystal X-ray of three chalcone derivatives, (2E)-3-(2-chlorophenyl) -1-(4-ethoxyphenyl) prop-2-en-1-one (**I**), (2E)-3-(3-chlorophenyl)-1-(4-ethoxyphenyl)prop-2-en-1-one (**II**) and (2E)-1-(4-ethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (**III**) was determined. The compound (**I**) crystallized in triclinic *P*-1 crystal system and in the asymmetric unit of the compound (**I**), two molecules were present. The conformational differences between molecule **A** and **B** indicated with the dihedral angles of 3.47 (2)° (**A**) and 8.12 (16)° (**B**), measured between chlorophenyl ring (C1A/B-C6A/B) and methoxy phenyl (C10A/B-C16A/B). Similarly the compound (**II**) crystallized in monoclinic *P*-1 crystal system and in the asymmetric unit of the compound (**II**), two molecules were crystallized. The conformational differences between molecule **A** and **B** with the dihedral angles of 4.50 (11)° (**A**) and 3.94 (11)° (**B**) was measured between terminal phenyl rings. The compound (**III**) crystallized in monoclinic, *P*21/*n*, with a dihedral angle between two terminal phenyl rings is 13.18 (7)°, indicating the near planarity of the compound. The intramolecular hydrogen bond of the types C---H...O is observed in all compounds (**I**), (**II**) and (**III**). In the crystal structures (**I**), (**II**) and (**III**), C---H... π intermolecular interaction was found in all compounds. The intermolecular hydrogen bond of the type C---H...O was present in compounds (**I**) and (**II**). The Hirshfeld surface analysis was carried for compounds (**I**), (**II**) and (**III**). Intercontacts C-C, C-H, C-O, H-H and O-H were common in all compounds which contributed more to the Hirshfeld surfaces. The electrostatic potential surfaces were drawn to understand electrophilic

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