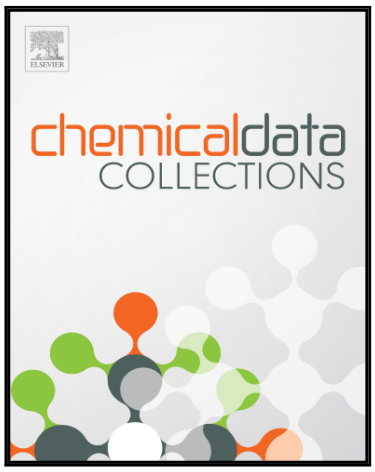

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Abstract

The title compounds (2E)-1-(4-2,4-dichlorophenyl)-3-[4-(propan-2-yl)phenyl]prop-2-en-1-one (**I**) and 2E)-1-(4-fluorophenyl)-3-[4-(propan-2-yl) phenyl]prop-2-en-1-one (**II**), have been synthesized by the base catalyzed Claisen-Schmidt condensation reaction of 4-(propan-2-yl)benzaldehyde with substituted acetophenones. The synthesized compounds were characterized by FT-IR, elemental analysis and single crystal X-ray diffraction. In **I** and **II**, the dihedral angle between the terminal rings are 54.68 $(19)^0$ and 53.42 $(8)^0$, respectively. The intra molecular hydrogen bond of the type C---H...O is observed in both the title compounds. The crystal structure is stabilized through C---O...π (**I**) and C---F...π (**II**) weak intermolecular interactions. Hirshfeld surfaces analysis computational method was carried to quantify the intermolecular interactions. The 2D finger print plots and electrostatic potential were plotted to evidence the intermolecular interactions.

Keywords Chalcones; Single crystal; Hirshfeld surface; Electrostatic potential; Finger print plots