

Synthesis and Phase Transition in New Chalcone Derivatives: Crystal Structure of 1-Phenyl-3-(4'-undecylcarbonyloxyphenyl)-2-propen-1-one

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A series of new chalcone derivatives with a general formula of $\text{CH}_3\text{C}_n\text{H}_{2n}\text{COOC}_6\text{H}_4\text{CH}:\text{CHCOC}_6\text{H}_4$ where $n = 10, 12, 14,$ and 16 were well synthesized and crystallized from organic solution. The physical properties as well as the chemical formulations of these compounds were determined by the microanalysis and spectroscopic methods (FTIR, and ^1H and ^{13}C NMR). Crystal structure of $\text{CH}_3\text{C}_{10}\text{H}_{20}\text{COOC}_6\text{H}_4\text{CH}:\text{CHCOC}_6\text{H}_4$ was determined by single-crystal X-ray diffraction analysis. The space group of this crystal is triclinic with $a = 5.8570(3) \text{ \AA}$, $b = 8.5640(5) \text{ \AA}$, $c = 24.1592(12) \text{ \AA}$, $V = 1175.82(11) \text{ \AA}^3$, and $Z = 2$, and its structure was refined to $R(F) = 0.055$ and $\omega R(F^2) = 0.161$. The elongated terminal alkyl chain is fully stretched in solid phase. Phase-transition temperatures and the thermal parameters were obtained from differential scanning calorimetry (DSC). The texture observation was carried out with a polarizing optical microscope (POM) over heating and cooling cycles. All of the title compounds except undecylcarbonyloxy analogue exhibit $\text{Cr}_1\text{-Cr}_2$ transition with smectic-like texture within the Cr_2 phase.

Keywords: chalcone derivatives; differential scanning calorimetry; 1-phenyl-3-(4'-undecylcarbonyloxyphenyl)-2-propen-1-one; polarizing optical microscope; single-crystal X-ray diffraction analysis

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