Title:	Design, synthesis and application of 2-chloro-3-nitrobenzoic acid based three-ring bent-core molecules with a terminal halogen moiety
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Keywords:	Bent core system Liquid crystal Luminescence Single crystal XRD
Issue Date:	2020
Publisher:	Elsevier
Citation:	Journal of Molecular Structure, 1202
Abstract:	Herein, we are reporting a new series of three-ring based polar bent-core molecules with 2-chloro-3-nitrobenzoic acid as the central core, halogen moiety at one terminal and octadecyloxy chain at another terminal. The compounds 10b, 10c, and 10d were shown to exhibit the orthogonal smectic phase during cooling the samples from the isotropic liquid. The mesomorphic behavior was characterized by polarizing optical microscope, differential scanning calorimetry, and small and wide-angle X-ray scattering experiment. All the compounds were shown to exhibit four peaks in the range of 400 nm–550 nm in emission spectra due to the combined effect of keto-enol tautomerism and excited-state intramolecular proton transfer (ESIPT) process along with solid-state luminescence property which can be useful for various applications like invisible ink. Crystal structure analysis along with density functional theory calculation reveals important structural parameters and packing of the molecular systems.
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