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Ragini Dubey, Rajasekhar Yerrasani, M. Karunakar, Angad Kumar Singh, Sandeep Kumar, T.R. Rao

PII: S0167-7322(17)34795-5

DOI: https://doi.org/10.1016/j.molliq.2017.12.067

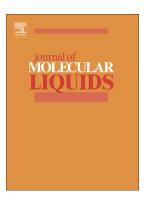
Reference: MOLLIQ 8363

To appear in: Journal of Molecular Liquids

Received date: 10 October 2017 Revised date: 29 November 2017 Accepted date: 12 December 2017

Please cite this article as: Ragini Dubey, Rajasekhar Yerrasani, M. Karunakar, Angad Kumar Singh, Sandeep Kumar, T.R. Rao, Synthesis, structural and mesophase characterization of isoindoline-1,3-dione based mesogenic Schiff bases. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), https://doi.org/10.1016/j.molliq.2017.12.067

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## **ACCEPTED MANUSCRIPT**

## [Revised Manuscript MOLLIQ\_2017\_4453\_R1]

Synthesis, Structural and Mesophase Characterization of Isoindoline-1,3-dione based Mesogenic Schiff Bases

Ragini Dubey<sup>1</sup>, Rajasekhar Yerrasani<sup>1</sup>, Karunakar M<sup>1</sup>., Angad Kumar Singh<sup>1</sup>, Sandeep Kumar<sup>2</sup> and T. R. Rao<sup>1</sup>\*

<sup>1</sup>Department of Chemistry, Banaras Hindu University, Varanasi-221005, India <sup>2</sup> Soft Condensed Matter Group, Raman Research Institute, Bangalore-560080, India \*Email: drtrrao@gmail.com

#### **Abstract**

Two homologous series of mesogenic Schiff-bases, [4-(((4-(1,3-dioxoisoindolin-2yl)phenyl)imino)methyl)-3-hydroxyphenyl-4-(alkoxy)benzoate,  $\mathrm{HL}_{1}^{n}$ , (Series I), which is an derivative 2-(4-((4-(alkoxy)-2ester of and hydroxybenzylidene)amino)phenyl)isoindoline-1,3-dione,  $HL_2^n$ , (Series II), which is an where  $HL = 2-\{4-[(2-Hydroxy-benzylidene)-amino]-phenyl\}$ alkoxy derivative of HL isoindole-1,3-dione) and  $n = -C_8H_{17}$ ,  $-C_{10}H_{21}$ ,  $-C_{12}H_{25}$  and  $-C_{14}H_{29}$ ] have been prepared and their molecular structures and thermal behaviour studied by FTIR, NMR and ESI-MS spectrometry, DSC, POM and variable temperature PXRD techniques; all these derivatives displayed an enantiotropic liquid crystalline behaviour with Nematic texture while few of them also exhibited SmA phase. Influence on thermal behaviour and mesomorphic properties upon changing the spacer was investigated in both the series. The HOMO and LUMO band gaps were found to be 2.89 and 3.26 eV for the two series respectively which were found to be in reasonable agreement with theoretical calculations (by DFT) made on optimized structure of one representative compound of each series.

**Keywords:** Liquid crystal; fluorescence; Isoindoline-1, 3-dione; Schiff-base.

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