Linear and Nonlinear Optical Properties of Indeno[2,1-b]fluorene and its Structural Isomers

Simil Thomas,* and Kwang S. Kim*

Supporting Information

Fig. 1 Geometry of indeno[2,1-b]fluorene (1) and it structural isomers used in the present study. The geometry is optimized at the UB3LYP/6-311G* level and all the systems have 20 $\pi$ electrons. Substituents attached at positions s and $s'$ are modelled with a different site energy.

![Fig. 1](image)

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2014

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2014

a Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan 689-798, Korea Fax: +82 52 217 5419; Tel: +82 52 217 5410; E-mail: kimks@unist.ac.kr