

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

Simil Thomas,^a and Kwang S. Kim^{*a}

Supporting Information

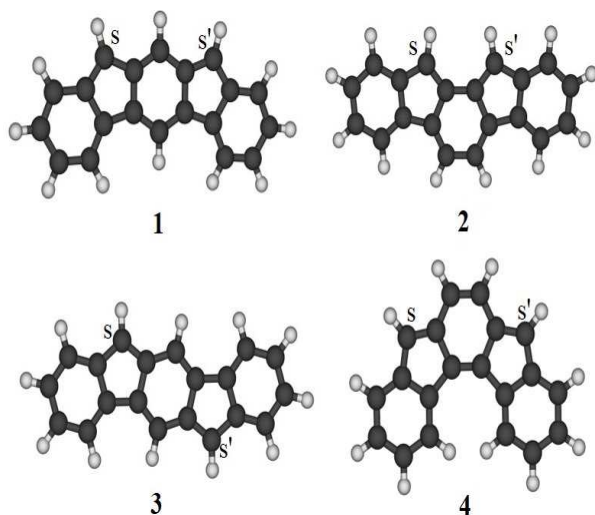


Fig. 1 Geometry of indeno[2,1-b]fluorene (**1**) and its structural isomers used in the present study. The geometry is optimized at the UB3LYP/6-311G* level and all the systems have 20 π electrons. Substituents attached at positions *s* and *s'* are modelled with a different site energy.

1

C 6.598315000 2.047456000 0 .000000000
 C 5.795635000 3.214546000 0 .000000000
 C 6.017631000 0.797539000 0 .000000000
 C 4.411722000 3.147392000 0 .000000000
 C 4.607899000 0.695947000 0 .000000000
 C 3.789384000 1.891328000 0 .000000000
 C 3.755755000 -0.425079000 0 .000000000
 C 2.413356000 1.480891000 0 .000000000
 C 2.412567000 0.035086000 0 .000000000
 C 1.212436000 -0.682728000 0 .000000000
 C 1.212436000 2.188732000 0 .000000000
 C 0.012305000 0.035086000 0 .000000000
 C 0.011515000 1.480891000 0 .000000000
 C -1.330883000 -0.425079000 0 .000000000

^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

C -1.364513000 1.891328000 0 .000000000
 C -2.183028000 0.695947000 0 .000000000
 C -1.986850000 3.147391000 0 .000000000
 C -3.592759000 0.797539000 0 .000000000
 C -3.370763000 3.214546000 0 .000000000
 C -4.173444000 2.047456000 0 .000000000
 H -1.398159000 4.059702000 0 .000000000
 H -3.856645000 4.185505000 0 .000000000
 H -5.253888000 2.146441000 0 .000000000
 H -4.206154000 -0.098602000 0 .000000000
 H -1.644459000 -1.462133000 0 .000000000
 H 1.212436000 -1.769930000 0 .000000000
 H 4.069330000 -1.462133000 0 .000000000
 H 6.631026000 -0.098602000 0 .000000000
 H 7.678760000 2.146441000 0 .000000000
 H 6.281516000 4.185505000 0 .000000000
 H 3.823030000 4.059702000 0 .000000000
 H 1.212436000 3.276027000 0 .000000000

2

C 4.652939000 0.726263000 0.000000000
 C 3.803220000 1.866046000 0.000000000
 C 2.421813000 1.369045000 0.000000000
 C 2.496319000 -0.098587000 0.000000000
 C 3.816927000 -0.467073000 0.000000000
 C 1.258847000 -0.840004000 0.000000000
 C -0.000235000 -0.082485000 0.000000000
 C -0.010510000 1.276808000 0.000000000
 C 1.228081000 2.019057000 0.000000000
 C -1.089798000 -1.065373000 0.000000000
 C -0.485512000 -2.352925000 0.000000000
 C 0.960934000 -2.178306000 0.000000000
 C 6.035371000 0.881956000 0.000000000
 C 4.339949000 3.143314000 0.000000000
 C -1.275124000 -3.498009000 0.000000000
 C -2.469276000 -0.936436000 0.000000000
 C 6.568629000 2.176119000 0.000000000
 C 5.734010000 3.292603000 0.000000000
 C -2.667752000 -3.357733000 0.000000000
 C -3.258614000 -2.095075000 0.000000000
 H -2.942110000 0.041308000 0.000000000
 H -4.340120000 -2.007111000 0.000000000

H -3.295519000 -4.243122000 0.000000000
H -0.824282000 -4.485850000 0.000000000
H -0.947231000 1.826022000 0.000000000
H 1.185531000 3.104108000 0.000000000
H 1.675758000 -2.992620000 0.000000000
H 4.197744000 -1.481445000 0.000000000
H 6.693495000 0.018352000 0.000000000
H 7.645459000 2.311806000 0.000000000
H 6.166487000 4.287779000 0.000000000
H 3.700832000 4.021366000 0.000000000

3

C -4.150191000 2.126201000 0.000000000
C -3.573414000 0.854199000 0.000000000
C -2.184120000 0.745972000 0.000000000
C -1.370959000 1.914937000 0.000000000
C -1.955089000 3.173121000 0.000000000
C -3.351457000 3.271828000 0.000000000
C -1.311420000 -0.415315000 0.000000000
C -0.002476000 0.001452000 0.000000000
C 0.026329000 1.469707000 0.000000000
C 1.203767000 2.148437000 0.000000000
C 2.427347000 1.398548000 0.000000000
C 2.398543000 -0.069707000 0.000000000
C 1.221104000 -0.748438000 0.000000000
C 3.795830000 -0.514937000 0.000000000
C 4.608991000 0.654027000 0.000000000
C 3.736291000 1.815315000 0.000000000
C 4.379961000 -1.773121000 0.000000000
C 5.998286000 0.545800000 0.000000000
C 5.776328000 -1.871828000 0.000000000
C 6.575062000 -0.726201000 0.000000000
H -4.200088000 -0.032615000 0.000000000
H -5.230803000 2.226549000 0.000000000
H -3.818968000 4.251184000 0.000000000
H -1.347546000 4.073248000 0.000000000
H 6.624960000 1.432615000 0.000000000
H 7.655674000 -0.826549000 0.000000000
H 6.243840000 -2.851185000 0.000000000
H 3.772417000 -2.673249000 0.000000000
H 4.075673000 2.844624000 0.000000000
H 1.186758000 -1.834590000 0.000000000
H 1.238113000 3.234590000 0.000000000
H -1.650802000 -1.444625000 0.000000000

4

C 6.571918000 -0.607679000 0.000000000
C 6.106931000 0.710877000 0.000000000
C 4.737193000 0.942919000 0.000000000
C 3.800948000 -0.132623000 0.000000000
C 4.286168000 -1.433113000 0.000000000
C 5.669521000 -1.665595000 0.000000000

C 2.444737000 0.472062000 0.000000000
C 2.665189000 1.939086000 0.000000000
C 4.005896000 2.195123000 0.000000000
C 1.156371000 0.009805000 0.000000000
C 0.053541000 1.002466000 0.000000000
C 0.301396000 2.416657000 0.000000000
C 1.575002000 2.873440000 0.000000000
C -1.144288000 0.347894000 0.000000000
C -0.912736000 -1.083947000 0.000000000
C 0.493660000 -1.318765000 0.000000000
C 0.946354000 -2.630863000 0.000000000
C 0.026675000 -3.690032000 0.000000000
C -1.342507000 -3.447427000 0.000000000
C -1.822244000 -2.134100000 0.000000000
H 1.998239000 -2.870266000 0.000000000
H 0.395170000 -4.710595000 0.000000000
H -2.040175000 -4.278714000 0.000000000
H -2.890098000 -1.937696000 0.000000000
H -2.121780000 0.815654000 0.000000000
H -0.543171000 3.098509000 0.000000000
H 1.793784000 3.936610000 0.000000000
H 4.462947000 3.177663000 0.000000000
H 6.806110000 1.541563000 0.000000000
H 7.638961000 -0.805630000 0.000000000
H 6.034201000 -2.687526000 0.000000000
H 3.626736000 -2.286942000 0.000000000