Supporting Information

Correlation between Solid-State Photophysical Properties and Molecular Packing in a Series of Indane-1,3-dione Containing Butadiene Derivatives

N. S. Saleesh Kumar †, Shinto Varghese†, C. H. Suresh‡, Nigam P. Rath§, Suresh Das *†

† Dr. Suresh Das, N. S. Saleesh Kumar, Shinto Varghese
Photosciences and Photonics Section
Chemical Sciences and Technology Division
National Institute for Interdisciplinary Science and Technology
Trivandrum – 695 019, Kerala, India,
Fax: (+) 91-471-2490186, E-mail: sureshdas55@gmail.com

‡ Computational Modeling and Simulation Section
National Institute for Interdisciplinary Science and Technology, CSIR, Trivandrum - 695 019, Kerala, India

§ Department of Chemistry and Biochemistry and Center for Nanoscience, University of Missouri-St. Louis, University of Missouri-St. Louis, MO 63121, USA.
Synthesis

The butadiene derivatives BINC8 and BINC12 were reported earlier\(^1\) and following the same synthetic procedures, lower derivatives BINC1 and BINC4 structures were established by FT-IR, \(^1\)H and \(^13\)C NMR. \(^1\)H NMR analysis revealed that the compounds existed as their \(E\) isomers.

\((E)-2-(3-(4-Methoxyphenyl)allylidene)-1H-indene-1,3(2H)-dione (BINC1):\) Orange yellow powder; 34%; mp: 220 °C; IR \(v_{\text{max}}\) (KBr): 3043, 2991, 2846, 2719, 1680, 1579, 1510, 1460, 1367, 1301, 1259, 1217, 1165, 1109, 1022, 989, 866, 817, 736, 601 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\), TMS): \(\delta\) 3.88 (s, 3H, -OCH\(_3\)), 6.95-6.96 (d, 2H, aromatic), 7.30-7.33 (d, 1H, vinylic, \(J = 15\) Hz), 7.63-7.66 (m, 3H, aromatic, vinylic), 7.77-7.79(m, 2H, aromatic), 7.95-7.97 (m, 2H, aromatic), 8.31-8.37 (dd, 1H, vinylic, \(J = 15.5\) Hz)) ppm; \(^13\)C NMR (75 MHz, CDCl\(_3\), TMS): \(\delta\) 55.46, 67.56, 114.60, 118.48, 121.72, 122.76, 122.96, 126.71, 128.52, 130.68, 134.76, 134.89, 142.13, 145.39, 151.44, 161.19, 182.30, 187.16, 190.30 ppm.

\((E)-2-(3-(4-Butoxyphenyl)allylidene)-1H-indene-1,3(2H)-dione (BINC4):\) Orange yellow powder; 40%; mp: 112 °C; IR (KBr) \(v_{\text{max}}\): 3053, 2954, 2873, 1714, 1674, 1571, 1510, 1469, 1371, 1317, 1249, 1279, 1166, 1105, 1039, 1010, 989, 842 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\), TMS): \(\delta\) 0.98-1.01 (t, 3H, CH\(_3\)), 1.49-1.53 (m, 2h,-CH\(_2\)-), 1.78-1.81 (m, 2H-ch\(_2\)- 4.01-4.04 (t, 2H, -OCH\(_2\)), 6.93-6.94 (d, 2H, aromatic), 7.29-7.32 (d, 1H, vinylic, \(J = 15\) Hz), 7.62-7.65 (m, 3H, aromatic,vinylic), 7.76-7.79 (m, 2H, aromatic), 7.94-7.96 (m, 2H, aromatic), 8.30-8.35 (dd, 1H, vinylic, \(J = 15.5\) Hz)) ppm; \(^13\)C NMR (75 MHz, CDCl\(_3\), TMS): \(\delta\) 13.89, 19.26, 31.24, 67.93, 96.19, 109.64, 112.48, 115.12, 121.67,
122.83, 123.02, 126.66, 128.36, 130.74, 134.69, 134.82, 140.91, 142.22, 145.47, 151.58, 161.89, 190.18, 190.63 ppm.

**Figure F1.** ORTEP diagram of BINC derivatives with a thermal ellipsoid probability of 50%.

**Figure F2.** Absorption spectra of: a) BINC1, b) BINC4, c) BINC8 and d) BINC12 in solution.
Figure F3. Diffuse reflectance absorption spectra of a) BINC1, b) BINC4, c) BINC8 and d) BINC12 in crystalline powders.

Table T1. Comparison of fluorescence lifetime data of BINC12 in crystalline and thin film forms.

<table>
<thead>
<tr>
<th>BINC12</th>
<th>Crystalline Powder</th>
<th>Thin film on slow cooling</th>
<th>Thin film on fast cooling</th>
</tr>
</thead>
<tbody>
<tr>
<td>τ(ns) / (%)</td>
<td>0.20 (75.30%)</td>
<td>1.93 (42.74%)</td>
<td>3.21 (51.95%)</td>
</tr>
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<td></td>
<td>0.48 (22.92%)</td>
<td>5.60 (34.90%)</td>
<td>6.67 (40.10%)</td>
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<td></td>
<td>3.81 (1.78%)</td>
<td>0.40 (22.35%)</td>
<td>0.84 (7.96%)</td>
</tr>
<tr>
<td>χ²</td>
<td>1.18</td>
<td>1.08</td>
<td>1.12</td>
</tr>
</tbody>
</table>
Figure F4. Expanded region of the aromatic part of NMR spectrum (500MHz) of BINC8 in CD$_3$CN solvent before, after irradiation and irradiated samples kept for 24 hours in dark.
Figure F5. NMR spectrum (500MHz) of BINC1 in CDCl$_3$ solvent.
Figure F6. NMR spectrum (500MHz) of BINC4 in CDCl₃ solvent.
Figure F7. NMR spectrum (500MHz) of **BINC8** in CDCl\textsubscript{3} solvent.
Figure F8. NMR spectrum (500MHz) of BINC12 in CDCl$_3$ solvent.

References