A comparison of homopolymer and block copolymer structure in 6FDA-based polyimides

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Partial charges were extracted via *ab initio* calculations at the B3LYP/6-31G** level for representative three-fragment structures based on the 6FDA dianhydride and the mPDA and durene diamines. The terms 6FDA_end, mPDA_end and durene_end stand for terminating groups.

![Diagram of 6FDA](image)

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
<th>i</th>
<th>j</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>mPDA-6FDA-mPDA</strong></td>
<td>-0.4475</td>
<td>0.6015</td>
<td>-0.0866</td>
<td>-0.0963</td>
<td>*</td>
<td>*</td>
<td>-0.4522</td>
<td>-0.1499</td>
<td>0.2291</td>
<td>-0.1488</td>
<td>-0.0964</td>
</tr>
<tr>
<td><strong>durene-6FDA-durene</strong></td>
<td>0.3200</td>
<td>0.3900</td>
<td>-0.1437</td>
<td>-0.1541</td>
<td>*</td>
<td>*</td>
<td>-0.4192</td>
<td>-0.0667</td>
<td>0.2690</td>
<td>-0.2098</td>
<td>-0.0112</td>
</tr>
<tr>
<td><strong>mPDA-6FDA-durene</strong></td>
<td>-0.3940</td>
<td>0.5944</td>
<td>-0.0344</td>
<td>-0.1361</td>
<td>*</td>
<td>*</td>
<td>-0.4308</td>
<td>-0.1911</td>
<td>0.2851</td>
<td>-0.1522</td>
<td>-0.0419</td>
</tr>
<tr>
<td><strong>l</strong></td>
<td>m</td>
<td>n</td>
<td>o</td>
<td>p</td>
<td>q</td>
<td>r</td>
<td>s</td>
<td>t</td>
<td>u</td>
<td>v</td>
<td></td>
</tr>
<tr>
<td><strong>mPDA-6FDA-mPDA</strong></td>
<td>0.1331</td>
<td>0.1420</td>
<td>0.1395</td>
<td>-0.4088</td>
<td>0.3855</td>
<td>-0.1085</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td><strong>durene-6FDA-durene</strong></td>
<td>0.1169</td>
<td>0.1462</td>
<td>0.1224</td>
<td>-0.5242</td>
<td>0.3704</td>
<td>-0.1014</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td><strong>mPDA-6FDA-durene</strong></td>
<td>0.1413</td>
<td>0.1500</td>
<td>0.1401</td>
<td>-0.5686</td>
<td>0.4292</td>
<td>-0.0992</td>
<td>0.2851</td>
<td>-0.0195</td>
<td>-0.1574</td>
<td>-0.1361</td>
<td>-0.0419</td>
</tr>
</tbody>
</table>
| **w**                | x | y | z | a' | b' | c' | d' | e'
| **mPDA-6FDA-mPDA**   | * | * | * | * | * | * | * | * |
| **durene-6FDA-durene** | * | * | * | * | * | * | * | * |
| **mPDA-6FDA-durene** | -0.1522 | 0.1413 | 0.1401 | 0.1500 | 0.1820 | 0.4628 | * | * | -0.4181 |

**Table S1.** Partial charges for 6FDA fragment.
<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
<th>i</th>
<th>J</th>
</tr>
</thead>
<tbody>
<tr>
<td>mPDA</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6FDA-mPDA-6FDA</td>
<td>-0.3793</td>
<td>0.4667</td>
<td>-0.4975</td>
<td>*</td>
<td>*</td>
<td>-0.0508</td>
<td>0.1893</td>
<td>0.2387</td>
<td>*</td>
<td>0.1098</td>
</tr>
</tbody>
</table>

**Table S2.** As table S1 for mPDA fragment.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>durene</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6FDA-durene-6FDA</td>
<td>-0.4137</td>
<td>0.1693</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>-0.2926</td>
<td>0.0876</td>
</tr>
</tbody>
</table>

**Table S3.** As table S1 for durene fragment.
**Table S4.** As table S1 for mPDA_end fragment.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
<th>i</th>
<th>j</th>
</tr>
</thead>
<tbody>
<tr>
<td>mPDA_end-6FDA-mPDA</td>
<td>-0.3289</td>
<td>0.4834</td>
<td>-0.4746</td>
<td>0.4020</td>
<td>-0.3559</td>
<td>-0.0176</td>
<td>0.1632</td>
<td>0.2099</td>
<td>0.1764</td>
<td>0.1230</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>k</th>
<th>l</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-0.7895</td>
<td>0.3250</td>
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</table>

**Table S5.** As table S1 for durene_end fragment.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>durene_end-6FDA-durene</td>
<td>0.3007</td>
<td>0.0132</td>
<td>0.1518</td>
<td>-0.6036</td>
<td>0*</td>
<td>0*</td>
<td>-0.3173</td>
<td>0.0966</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>i</th>
<th>j</th>
<th>k</th>
<th>l</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-0.3034</td>
<td>0.0981</td>
<td>-0.8647</td>
<td>0.3490</td>
</tr>
<tr>
<td></td>
<td>a</td>
<td>b</td>
<td>c</td>
<td>d</td>
</tr>
<tr>
<td>------------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td><strong>6FDA_end</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6FDA-mPDA-6FDA_end</td>
<td>-0.4054</td>
<td>0.5418</td>
<td>-0.0342</td>
<td>-0.1307</td>
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<tr>
<td>6FDA-durene-6FDA_end</td>
<td>-0.3932</td>
<td>0.5571</td>
<td>-0.0219</td>
<td>-0.1185</td>
</tr>
<tr>
<td>l</td>
<td></td>
<td>m</td>
<td>n</td>
<td>o</td>
</tr>
<tr>
<td>6FDA-mPDA-6FDA_end</td>
<td>0.1380</td>
<td>0.1448</td>
<td>0.1388</td>
<td>-0.5365</td>
</tr>
<tr>
<td>6FDA-durene-6FDA_end</td>
<td>0.1503</td>
<td>0.1571</td>
<td>0.1511</td>
<td>-0.5243</td>
</tr>
<tr>
<td>w</td>
<td></td>
<td>x</td>
<td>y</td>
<td>z</td>
</tr>
<tr>
<td>6FDA-mPDA-6FDA_end</td>
<td>-0.1335</td>
<td>0.1293</td>
<td>0.1450</td>
<td>0.1308</td>
</tr>
<tr>
<td>6FDA-durene-6FDA_end</td>
<td>-0.1212</td>
<td>0.1415</td>
<td>0.1573</td>
<td>0.1430</td>
</tr>
</tbody>
</table>

**Table S6.** As table S1 for 6FDA_end fragment.