Supporting Information

New low bandgap near-IR conjugated D-A copolymers for BHJ polymers solar cell applications


*Institute of Organoelement Compounds of the Russian Academy of Sciences, Vavilova St., 28, 119991 Moscow, Russian Federation
bCarl von Ossietzky University of Oldenburg, 26129, Oldenburg, Germany
cLomonosov Moscow State University, Faculty of Physics, 1-2 Leninskiye Gory, Moscow 119991, Russian Federation
dInstitute of Organic Chemistry of the Russian Academy of Sciences, Leninsky prospect 47, 119991 Moscow, Russian Federation
eMolecular Engineering Laboratory, Department of Physics, University of Patras, Patras, 26500 GR, Greece
fDepartment of Electronics and communication Engineering, LNMIIT (Deemed University), Jamdoli, Jaipur (Raj.) 302031, India
gMolecular Electronics and Optoelectronics Device Research Laboratory, Department of Physics, LNMIIT (Deemed University), Jamdoli, Jaipur (Raj.) 302031, India

Figure S1Total and partial density of states of (a) P1, and (b) P2 (calculated using the M06 functional).
Figure S2 Theoretical UV/Vis absorption spectrum of (a) P1, and (b) P2 (calculated using the B3LYP functional).
Table S1: Electronic excitations of P1 (with non-negligible oscillator strengths, $f$), and the corresponding major contributions. Calculated using the M06 functional (and CF for solvent).

<table>
<thead>
<tr>
<th>No.</th>
<th>Wavelength (nm)</th>
<th>$f$</th>
<th>Main Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>788</td>
<td>0.350</td>
<td>H→L (99%)</td>
</tr>
<tr>
<td>2</td>
<td>584</td>
<td>0.029</td>
<td>H→1→L (93%)</td>
</tr>
<tr>
<td>3</td>
<td>485</td>
<td>0.053</td>
<td>H→3→L (10%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→2→L (83%)</td>
</tr>
<tr>
<td>4</td>
<td>447</td>
<td>0.036</td>
<td>H→3→L (86%)</td>
</tr>
<tr>
<td>5</td>
<td>434</td>
<td>0.339</td>
<td>H→L+1 (95%)</td>
</tr>
<tr>
<td>6</td>
<td>407</td>
<td>0.162</td>
<td>H→L+2 (93%)</td>
</tr>
<tr>
<td>7</td>
<td>390</td>
<td>0.125</td>
<td>H→4→L (66%)</td>
</tr>
<tr>
<td>8</td>
<td>385</td>
<td>0.093</td>
<td>H→6→L (73%)</td>
</tr>
<tr>
<td>9</td>
<td>372</td>
<td>0.081</td>
<td>H→8→L (10%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→7→L (55%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→1→L+1 (23%)</td>
</tr>
<tr>
<td>10</td>
<td>370</td>
<td>0.157</td>
<td>H→7→L (15%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→1→L+1 (70%)</td>
</tr>
<tr>
<td>11</td>
<td>341</td>
<td>0.025</td>
<td>H→8→L (61%)</td>
</tr>
<tr>
<td>12</td>
<td>337</td>
<td>0.036</td>
<td>H→1→L+2 (17%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+3 (62%)</td>
</tr>
<tr>
<td>13</td>
<td>333</td>
<td>0.143</td>
<td>H→1→L+2 (68%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+3 (20%)</td>
</tr>
<tr>
<td>14</td>
<td>327</td>
<td>0.253</td>
<td>H→2→L+1 (40%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+4 (35%)</td>
</tr>
<tr>
<td>15</td>
<td>323</td>
<td>0.595</td>
<td>H→2→L+1 (42%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+4 (27%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+5 (15%)</td>
</tr>
<tr>
<td>16</td>
<td>315</td>
<td>0.566</td>
<td>H→L+4 (13%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+5 (61%)</td>
</tr>
<tr>
<td>17</td>
<td>302</td>
<td>0.026</td>
<td>H→18→L (43%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→17→L (11%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→10→L (11%)</td>
</tr>
<tr>
<td>18</td>
<td>298</td>
<td>0.026</td>
<td>H→10→L (69%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→2→L+2 (12%)</td>
</tr>
<tr>
<td>19</td>
<td>298</td>
<td>0.151</td>
<td>H→10→L (14%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→2→L+2 (53%)</td>
</tr>
<tr>
<td>20</td>
<td>285</td>
<td>0.121</td>
<td>H→15→L (39%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→13→L (36%)</td>
</tr>
<tr>
<td>21</td>
<td>283</td>
<td>0.296</td>
<td>H→15→L (28%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→14→L (27%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→13→L (23%)</td>
</tr>
<tr>
<td>22</td>
<td>281</td>
<td>0.040</td>
<td>H→3→L+2 (14%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→1→L+3 (24%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H→L+7 (12%)</td>
</tr>
</tbody>
</table>
Table S2 Electronic excitations of P2 (with non-negligible oscillator strengths, $f$), and the corresponding major contributions. Calculated using the M06 functional (and CF for solvent).

<table>
<thead>
<tr>
<th>No.</th>
<th>Wavelength (nm)</th>
<th>$f$</th>
<th>Main Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>800</td>
<td>0.381</td>
<td>H→L (99%)</td>
</tr>
<tr>
<td>2</td>
<td>588</td>
<td>0.037</td>
<td>H→L+1 (96%)</td>
</tr>
<tr>
<td>3</td>
<td>463</td>
<td>0.037</td>
<td>H→L (94%)</td>
</tr>
<tr>
<td>4</td>
<td>440</td>
<td>0.462</td>
<td>H→L+1 (92%)</td>
</tr>
<tr>
<td>5</td>
<td>412</td>
<td>0.130</td>
<td>H→L+2 (89%)</td>
</tr>
<tr>
<td>6</td>
<td>407</td>
<td>0.081</td>
<td>H→L (85%)</td>
</tr>
<tr>
<td>7</td>
<td>396</td>
<td>0.047</td>
<td>H→L (26%)</td>
</tr>
<tr>
<td>8</td>
<td>385</td>
<td>0.100</td>
<td>H→L (65%)</td>
</tr>
<tr>
<td>9</td>
<td>377</td>
<td>0.042</td>
<td>H→L (73%)</td>
</tr>
<tr>
<td>10</td>
<td>370</td>
<td>0.193</td>
<td>H→L+1 (87%)</td>
</tr>
<tr>
<td>12</td>
<td>347</td>
<td>0.124</td>
<td>H→L+3 (89%)</td>
</tr>
<tr>
<td>13</td>
<td>336</td>
<td>0.158</td>
<td>H→L+2 (77%)</td>
</tr>
<tr>
<td>14</td>
<td>329</td>
<td>0.228</td>
<td>H→L+4 (11%)</td>
</tr>
<tr>
<td>15</td>
<td>328</td>
<td>0.513</td>
<td>H→L+4 (24%)</td>
</tr>
<tr>
<td>16</td>
<td>325</td>
<td>0.064</td>
<td>H→L+5 (78%)</td>
</tr>
<tr>
<td>18</td>
<td>304</td>
<td>0.127</td>
<td>H→L+1 (21%)</td>
</tr>
<tr>
<td>19</td>
<td>302</td>
<td>0.139</td>
<td>H→L (15%)</td>
</tr>
<tr>
<td>21</td>
<td>296</td>
<td>0.145</td>
<td>H→L+1 (48%)</td>
</tr>
<tr>
<td>22</td>
<td>294</td>
<td>0.031</td>
<td>H→L+1 (20%)</td>
</tr>
<tr>
<td>24</td>
<td>288</td>
<td>0.084</td>
<td>H→L+2 (65%)</td>
</tr>
<tr>
<td>26</td>
<td>284</td>
<td>0.034</td>
<td>H→L+4 (15%)</td>
</tr>
<tr>
<td>27</td>
<td>283</td>
<td>0.339</td>
<td>H→L (15%)</td>
</tr>
</tbody>
</table>