Supporting Information

Electronic structures and optical properties of the IPR-violating C_{60}X_8 (X=H, F, and Cl) fullerene compounds: A computational study

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Table S1. Pyramidalization angles (degree) of the $sp^2$ carbon atoms in $C_{60}$ ($C_{2v}$) and $C_{60}X_8$ (X=H, F, and Cl).

<table>
<thead>
<tr>
<th>Carbon atoms</th>
<th>Pyramidalization angle (deg.)</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$C_{60}$ ($C_{2v}$)</td>
</tr>
<tr>
<td>1, 5, 8, 9</td>
<td>12.35</td>
</tr>
<tr>
<td>2, 6, 36, 42</td>
<td>11.42</td>
</tr>
<tr>
<td>3, 7, 21, 22</td>
<td>8.67</td>
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<tr>
<td>4, 17, 46, 50</td>
<td>12.91</td>
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<tr>
<td>10, 19, 30, 55</td>
<td>10.90</td>
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<tr>
<td>11, 15, 18, 25</td>
<td>11.69</td>
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<tr>
<td>12, 24</td>
<td>12.44</td>
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<tr>
<td>13, 16, 40, 47</td>
<td>14.88</td>
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<td>11.14</td>
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<td>26, 28</td>
<td>11.28</td>
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<td>32, 38, 41, 54</td>
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<td>43, 51, 58, 60</td>
<td>11.57</td>
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<td>45, 48, 52, 56</td>
<td>11.76</td>
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<tr>
<td>57, 59</td>
<td>11.66</td>
</tr>
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</table>
Table S2. The NICS values at all pentagon and hexagon ring centers, as well as values 1.0 Å above [NICS(1)] and below [NICS(-1)] each ring of two separate conjugated annulene subunits in $C_{60}X_8$ (X=H, F and Cl).

<table>
<thead>
<tr>
<th>NICS(ppm)</th>
<th>A'</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
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<tbody>
<tr>
<td>$C_{60}$ ($C_{2v}$)</td>
<td>4.7(1)</td>
<td>0.0 (1)</td>
<td>4.3(1)</td>
<td>-0.3(1)</td>
<td>0.4(1)</td>
<td>7.2(1)</td>
<td>0.3(1)</td>
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<tr>
<td></td>
<td>7.2(0)</td>
<td>-1.8(0)</td>
<td>7.6(0)</td>
<td>-2.3(0)</td>
<td>-1.6(0)</td>
<td>13.8(0)</td>
<td>0.0(0)</td>
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<tr>
<td></td>
<td>3.4(-1)</td>
<td>-3.2(-1)</td>
<td>3.4(-1)</td>
<td>-4.4(-1)</td>
<td>-3.8(-1)</td>
<td>4.6(-1)</td>
<td>-2.3(-1)</td>
</tr>
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<td>$C_{60}H_8$</td>
<td>-6.6(1)</td>
<td>-4.4(1)</td>
<td>1.5(1)</td>
<td>-1.9(1)</td>
<td>-2.2(1)</td>
<td>3.4(1)</td>
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<td>-10.9(0)</td>
<td>-11.0(0)</td>
<td>1.6(0)</td>
<td>-7.8(0)</td>
<td>-8.5(0)</td>
<td>4.7(0)</td>
<td>-11.3(0)</td>
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<tr>
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<td>-18.5(-1)</td>
<td>-19.4(-1)</td>
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<td>-11.5(0)</td>
<td>-11.2(0)</td>
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<td>-8.2(0)</td>
<td>-8.8(0)</td>
<td>3.8(0)</td>
<td>-11.2(0)</td>
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<tr>
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<td>-18.8(-1)</td>
<td>-20.0(-1)</td>
<td>-14.4(-1)</td>
<td>-20.0(-1)</td>
<td>-20.8(-1)</td>
<td>-13.5(-1)</td>
<td>-20.2(-1)</td>
</tr>
<tr>
<td>$C_{60}Cl_8$</td>
<td>-6.3(1)</td>
<td>-4.7(1)</td>
<td>1.2(1)</td>
<td>-2.1(1)</td>
<td>-2.4(1)</td>
<td>3.1(1)</td>
<td>-4.4(1)</td>
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<tr>
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<td>-11.7(0)</td>
<td>-11.5(0)</td>
<td>0.9(0)</td>
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<td>-8.8(0)</td>
<td>3.9(0)</td>
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<tr>
<td></td>
<td>-18.3(-1)</td>
<td>-19.8(-1)</td>
<td>-14.2(-1)</td>
<td>-19.8(-1)</td>
<td>-20.5(-1)</td>
<td>-13.2(-1)</td>
<td>-20.2(0)</td>
</tr>
</tbody>
</table>
Table S3. TD-DFT (B3LYP) calculated excitation energies ($\Delta E$), oscillator strengths ($f_{osc}$), the largest coefficients in the configurational interaction (CI) expansions, and major transition composition with $f_{osc}>0.100$ of C$_{60}$ ($C_{2v}$) and C$_{60}X_8$ compounds, in which the H and L refer to HOMO and LUMO.

<table>
<thead>
<tr>
<th>State</th>
<th>Sym.</th>
<th>$\Delta E$(eV)(nm)</th>
<th>$f_{osc}$</th>
<th>CI coefficient</th>
<th>Major configuration</th>
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<tbody>
<tr>
<td>$E_{111}$</td>
<td>$B_1$</td>
<td>4.83 (256.9)</td>
<td>0.1351</td>
<td>0.43075</td>
<td>H-3→L+12 (37%)</td>
</tr>
<tr>
<td>$E_{124}$</td>
<td>$A_1$</td>
<td>5.01 (247.0)</td>
<td>0.4420</td>
<td>0.40117</td>
<td>H-1→L+12 (32%)</td>
</tr>
<tr>
<td>$E_{135}$</td>
<td>$B_2$</td>
<td>4.94 (238.2)</td>
<td>0.2697</td>
<td>0.43524</td>
<td>H-6→L+5 (38%)</td>
</tr>
<tr>
<td>$E_{166}$</td>
<td>$B_2$</td>
<td>5.52 (224.6)</td>
<td>0.1166</td>
<td>0.45624</td>
<td>H-5→L+12 (42%)</td>
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<tr>
<td>$E_{225}$</td>
<td>$B_2$</td>
<td>5.95 (208.0)</td>
<td>0.1340</td>
<td>0.43857</td>
<td>H→L+17 (38%)</td>
</tr>
<tr>
<td>$E_{231}$</td>
<td>$B_2$</td>
<td>6.00 (206.5)</td>
<td>0.3340</td>
<td>0.35888</td>
<td>H→L+17 (26%)</td>
</tr>
<tr>
<td>$E_{233}$</td>
<td>$A_1$</td>
<td>6.01 (206.2)</td>
<td>0.1483</td>
<td>0.26012</td>
<td>H-12→L+11 (14%)</td>
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<tr>
<td>$E_{234}$</td>
<td>$B_2$</td>
<td>5.56 (205.7)</td>
<td>0.1513</td>
<td>0.36306</td>
<td>H-14→L+3 (26%)</td>
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<tr>
<td>$E_{236}$</td>
<td>$B_1$</td>
<td>5.58 (205.4)</td>
<td>0.3975</td>
<td>0.42218</td>
<td>H-11→L+10 (36%)</td>
</tr>
<tr>
<td>$E_{238}$</td>
<td>$B_2$</td>
<td>6.06 (204.4)</td>
<td>0.1096</td>
<td>0.29097</td>
<td>H-7→L+17 (38%)</td>
</tr>
<tr>
<td>$E_{242}$</td>
<td>$A_1$</td>
<td>6.09 (203.3)</td>
<td>0.2043</td>
<td>0.36966</td>
<td>H-12→L+11 (27%)</td>
</tr>
<tr>
<td>$E_{256}$</td>
<td>$B_2$</td>
<td>6.23 (198.9)</td>
<td>0.1102</td>
<td>0.43649</td>
<td>H-28→L+2 (38%)</td>
</tr>
<tr>
<td>$E_{270}$</td>
<td>$B_1$</td>
<td>6.34 (195.5)</td>
<td>0.1749</td>
<td>0.37469</td>
<td>H-1→L+18 (28%)</td>
</tr>
<tr>
<td>$E_{276}$</td>
<td>$B_1$</td>
<td>6.37 (194.5)</td>
<td>0.1115</td>
<td>0.44636</td>
<td>H-21→L+3 (40%)</td>
</tr>
<tr>
<td>$E_{301}$</td>
<td>$A_1$</td>
<td>6.57 (188.6)</td>
<td>0.1592</td>
<td>0.37134</td>
<td>H-2→L+20 (28%)</td>
</tr>
</tbody>
</table>

C$_{60}$H$_8$

| $E_{102}$ | $B_1$ | 5.14 (241.0) | 0.1334 | 0.48403 | H-6→L+6 (47%) |
| $E_{109}$ | $B_1$ | 5.27 (235.4) | 0.2723 | 0.44830 | H-6→L+6 (40%) |
| $E_{164}$ | $B_1$ | 5.90 (209.3) | 0.1008 | 0.48999 | H-22→L+1 (28%) |
| $E_{173}$ | $B_1$ | 5.98 (207.4) | 0.2419 | 0.37129 | H-22→L+1 (28%) |
| $E_{214}$ | $A_1$ | 6.39 (194.1) | 0.1126 | 0.46351 | H-18→L+2 (43%) |
| $E_{215}$ | $B_1$ | 6.42 (193.1) | 0.1235 | 0.52194 | H-8→L+13 (54%) |
| $E_{233}$ | $A_1$ | 6.56 (189.1) | 0.1663 | 0.50269 | H→L+17 (51%) |
| $E_{257}$ | $B_2$ | 6.79 (182.7) | 0.1525 | 0.36155 | H-2→L+16 (26%) |
| $E_{300}$ | $A_1$ | 7.12 (174.2) | 0.1119 | 0.47861 | H-14→L+7 (46%) |

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\[
\begin{array}{llllll}
\text{C}_{60}\text{F}_8 & & & & & \\
E_{71} & B_2 & 4.58 \ (270.4) & 0.2025 & 0.37786 & H \rightarrow L+9 \ (29\%)
\\
E_{78} & B_1 & 4.69 \ (264.2) & 0.1029 & 0.49619 & H \rightarrow L+10 \ (49\%)
\\
E_{100} & A_1 & 5.02 \ (246.6) & 0.1017 & 0.31622 & H-1 \rightarrow L+10 \ (20\%)
\\
E_{131} & B_1 & 5.35 \ (231.4) & 0.1227 & 0.42332 & H-11 \rightarrow L+3 \ (36\%)
\\
E_{205} & B_1 & 5.98 \ (207.3) & 0.3078 & 0.03938 & H-6 \rightarrow L+12 \ (28\%)
\\
E_{241} & A_1 & 6.24 \ (198.7) & 0.2395 & 0.29274 & H-11 \rightarrow L+10 \ (20\%)
\\
E_{254} & B_1 & 6.35 \ (195.1) & 0.2399 & 0.51345 & H-8 \rightarrow L+13 \ (53\%)
\\
E_{278} & A_1 & 6.51 \ (190.5) & 0.1069 & 0.56749 & H-10 \rightarrow L+11 \ (64\%)
\\
E_{302} & A_1 & 6.68 \ (185.6) & 0.1002 & 0.52113 & H-26 \rightarrow L+4 \ (54\%)
\\
\end{array}
\]

\[
\begin{array}{llllll}
\text{C}_{60}\text{Cl}_8 & & & & & \\
E_{89} & B_2 & 4.57 \ (271.0) & 0.1330 & 0.59724 & H-9 \rightarrow L+3 \ (71\%)
\\
E_{170} & B_1 & 5.14 \ (241.1) & 0.1576 & 0.37613 & H-4 \rightarrow L+10 \ (28\%)
\\
E_{184} & B_2 & 5.23 \ (236.8) & 0.1084 & 0.49039 & H-10 \rightarrow L+6 \ (48\%)
\\
E_{242} & A_1 & 5.61 \ (220.6) & 0.1349 & 0.27969 & H-29 \rightarrow L+1 \ (29\%)
\\
E_{264} & B_1 & 5.78 \ (214.5) & 0.1618 & 0.36658 & H-6 \rightarrow L+12 \ (27\%)
\\
E_{265} & B_2 & 5.78 \ (214.3) & 0.1059 & 0.39574 & H-29 \rightarrow L+2 \ (31\%)
\\
E_{275} & B_2 & 5.84 \ (212.3) & 0.1145 & 0.35545 & H-31 \rightarrow L+1 \ (25\%)
\\
E_{280} & B_1 & 5.86 \ (211.4) & 0.1011 & 0.39401 & H-35 \rightarrow L \ (31\%)
\\
E_{332} & B_1 & 6.19 \ (200.3) & 0.1350 & 0.36880 & H-8 \rightarrow L+13 \ (27\%)
\\
E_{335} & B_2 & 6.20 \ (200.1) & 0.1453 & 0.37301 & H-38 \rightarrow L \ (28\%)
\\
\end{array}
\]