**Organic Electronics**

- Potential alternations from conventional inorganic devices
- Promising applications to organic light-emitting diodes, organic solar cells, and organic field-effect transistors, due to their low cost, light weight, and flexible devices.

*(Images from http://www.lg.com)*

**Highly Extended \(\pi\)-Conjugated Organic Molecules**

Most of such molecules possess unique features, such as a rigid structural motif and an abundant \(\pi\) electrons.

![DFT Calculations](image)

DFT calculations were carried out using Gaussian 09 program at the B3LYP/6-311G+ (d,p) levels of theory as a basis set. 

\(\mu \|\) : Dipole moment in a longer axis estimated by the DFT calculation.

\[
\begin{align*}
1: \text{HOMO: } & -5.86 \text{ eV} \\
\mu\| & = 5.62 \text{ Debye}
\end{align*}
\]

\[
\begin{align*}
2: \text{HOMO: } & -5.78 \text{ eV} \\
\mu\| & = 6.04 \text{ Debye}
\end{align*}
\]

\[
\begin{align*}
3: \text{HOMO: } & -5.58 \text{ eV} \\
\mu\| & = 1.54 \text{ Debye}
\end{align*}
\]

\[
\begin{align*}
B: \text{HOMO: } & -5.80 \text{ eV} \\
\mu\| & = 0.00 \text{ Debye}
\end{align*}
\]

**Phase Transition Behavior**

<table>
<thead>
<tr>
<th>Heating</th>
<th>Cooling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal</td>
<td>149</td>
</tr>
<tr>
<td>Nematic (LC)</td>
<td>140</td>
</tr>
<tr>
<td>Liquid</td>
<td>225</td>
</tr>
</tbody>
</table>

Determined by DSC or POM.

**POM image**

1. Heating
2. Cooling
3. Heating
4. Cooling

- Donor-acceptor structure attributed to the increase of their clearing point.
- "OMe" at the terminal may play important role to appear LC phases.

**Photophysical Properties**

*(Solution-state (CH\(_2\)Cl\(_2\), 10\(^{-6}\)M))*

- Photoluminescence in both solution and solid-states
- Emission behaviors were changed between in solution and in solid states.
  - PL depends on aggregated structures of the molecules.
  - Emissive in even LC phase
  - Reversible PL behaviors between solid and LC phases.

**Crystal Packing Structure of 1**

- CH/\(\pi\) interaction 2.95 Å (CH–\(\pi\))
- \(\pi\)/\(\pi\) interaction 3.41 Å (\(\pi\)-\(\pi\))
- van der Waals radii: C, 1.70 Å; H, 1.20 Å; F, 1.50 Å.
- Pentafluorophenyl (C\(_5\)F\(_5\)) moiety in 1 affected to construct a relatively loose packing to easily generate LC phase; Lower melting point

**Conclusion**

- We found several 1,4-bis(phenylethynyl)benzene derivatives exhibited not only LC behavior but also photoluminescence in solution, solid state, and even LC phase.
- Precise structural design was important to gain desired properties.

**Acknowledgement**

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**In This Study...**

We would develop new light-emitting liquid-crystalline (LELC) materials with both LC and light-emitting properties.

- Molecule Design:
- Rod-shaped rigid motif for LC property
- Extended \(\pi\)-conjugation for LE property
- Electron-donating and withdrawing substituents for the alignment control

**Crystal Packing Structure of 1**

- Hydrogen bonding 2.56 Å (H–F)
- \(\pi\)/\(\pi\) interaction 3.41 Å (\(\pi\)-\(\pi\))
- Pentafluorophenyl (C\(_5\)F\(_5\)) moiety in 1 affected to construct a relatively loose packing to easily generate LC phase; Lower melting point