Covalent Organic Frameworks Anchored with Frustrated Lewis Pairs for Hydrogenation of Alkynes with H₂

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1. Results and discussion

![FT-IR spectra](image)

Figure S1. The FT-IR spectra of COFs-1, COFs-1-PPh₂, COFs-2, COFs-2-PPh₂ and PPh₃.
Figure S2. The EDX mapping images of COFs-1, COFs-1-PPh\(_2\), COFs-2 and COFs-2-PPh\(_2\).

Table S1. Elemental contents of COFs-1, COFs-2, COFs-1-PPh\(_2\) and COFs-2-PPh\(_2\).

<table>
<thead>
<tr>
<th></th>
<th>C(^{[a]})</th>
<th>H(^{[a]})</th>
<th>N(^{[a]})</th>
<th>Br(^{[b]})</th>
<th>P(^{[b]})</th>
<th>Cu(^{[b]})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(wt%)</td>
<td>(wt%)</td>
<td>(wt%)</td>
<td>(wt%)</td>
<td>(wt%)</td>
<td>(wt%)</td>
</tr>
<tr>
<td>COFs-1</td>
<td>Exp. 52.8</td>
<td>2.5</td>
<td>10.9</td>
<td>30.5±4.2</td>
<td>~</td>
<td>~</td>
</tr>
<tr>
<td></td>
<td>Theo. 53.7</td>
<td>2.4</td>
<td>11.4</td>
<td>32.5</td>
<td>~</td>
<td>~</td>
</tr>
<tr>
<td>COFs-1-PPh(_2)</td>
<td>Exp. 70.6</td>
<td>4.6</td>
<td>9.8</td>
<td>14.3±3.1</td>
<td>4.7±1.1</td>
<td>0.05±0.01</td>
</tr>
<tr>
<td></td>
<td>Theo. 78.6</td>
<td>4.6</td>
<td>8.0</td>
<td>0</td>
<td>8.8</td>
<td>~</td>
</tr>
<tr>
<td>COFs-2</td>
<td>Exp. 57.8</td>
<td>2.7</td>
<td>5.6</td>
<td>31.2±5.1</td>
<td>~</td>
<td>~</td>
</tr>
<tr>
<td></td>
<td>Theo. 58.8</td>
<td>2.9</td>
<td>5.7</td>
<td>32.7</td>
<td>~</td>
<td>~</td>
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<tr>
<td>COFs-2-PPh(_2)</td>
<td>Exp. 68.1</td>
<td>4.7</td>
<td>5.3</td>
<td>8.9±1.9</td>
<td>3.5±0.8</td>
<td>0.08±0.02</td>
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<tr>
<td></td>
<td>Theo. 82.3</td>
<td>4.9</td>
<td>4.0</td>
<td>0</td>
<td>8.9</td>
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\(^{[a]}\) Determined by elemental analyses. \(^{[b]}\) Determined by EDX equipped on SEM (Take the average of the five tests).
Figure S3. TGA of COFs-1, COFs-1-PPh₂, COFs-2 and COFs-2-PPh₂.
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Table S2. Investigation of COFs/BCF, COFs-FLPs and Br-free-COFs-1-P/BCF in the catalytic hydrogenation of 5-decyne to Z-5-decene.

<table>
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<th>Entry</th>
<th>Catalyst</th>
<th>T/h</th>
<th>Conversion/%</th>
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<tr>
<td>1</td>
<td>COFs-1/BCF</td>
<td>48</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>COFs-2/BCF</td>
<td>48</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>COFs-1-FLPs</td>
<td>36</td>
<td>88</td>
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<tr>
<td>4</td>
<td>COFs-2-FLPs</td>
<td>36</td>
<td>87</td>
</tr>
<tr>
<td>5</td>
<td>Br-free-COFs-1-P/BCF</td>
<td>48</td>
<td>14</td>
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Figure S18. PXRD of COFs-1-FLPs and COFs-2-FLPs after 10 runs.

Figure S19. $^{13}$C NMR spectrum of BCF (in CDCl$_3$, 101 MHz).
Figure S20. $^{19}$F NMR spectrum of BCF (in CDCl$_3$, 376 MHz).

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Figure S22. Simulated theoretical PXRD patterns of COFs-1 and COFs-1-PPh$_2$. (Br was completely replaced by -PPh$_2$)

2. Original MS data

1.
2. 
\[ (\text{CH}_2)_2 \ (\text{H}_2\text{C})_2 \]

3. 
\[ (\text{CH}_2)_2 \ (\text{H}_2\text{C})_2 \]
4. 

\[ (\text{CH}_2)_3 \quad (\text{H}_2\text{C})_3 \]

5. 

\[ (\text{H}_2\text{C})_4 \quad (\text{H}_2\text{C})_4 \]
6.

![Graph](image1)

7.

![Graph](image2)
12. \[
\begin{align*}
\text{Ph} & \quad \text{Cl}
\end{align*}
\]

13. \[
\begin{align*}
\text{Ph} & \quad \text{Ph}
\end{align*}
\]
Reference: