MATERIAL SUPLEMENTAR

Self-assembly and host-guest behaviors of a supramolecular helicate Fe^{II}_{2}L_{3}

Xiao-Huan Fu, Wen-Yuan Wu*, Peng Jiang, Zhen-Yu Han, and Rong Wan#

College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211800, P. R. China

Recebido em 03/12/2017; aceito em 23/02/2018; publicado na web em
COM MATERIAL SUPLEMENTAR

*e-mail: wwy@njtech.edu.cn

#alternative e-mail: rwan@njtech.edu.cn
\(^1\)H NMR SPECTRUM OF SUBCOMPONENT TRIAMINE

Figure 1S. \(^1\)H NMR spectrum of subcomponent triamine in CD₃CN at 293 K
\textbf{1H NMR SPECTRUMS OF HOST-GUEST INTERACTIONS}

\textbf{Figure 2S.} $^1$H NMR spectrum of helicate 1 with pyrene in CD$_3$CN at 293 K

\textbf{Figure 3S.} $^1$H NMR spectrum of pyrene in CD$_3$CN at 293 K
Figure 4S. $^1$H NMR spectrum of helicate 1 with naphthalene-1,5-diol in CD$_3$CN at 293 K

Figure 5S. $^1$H NMR spectrum of naphthalene-1,5-diol in CD$_3$CN at 293 K
Figure 6S. $^1$H NMR spectrum of helicate 1 with 1,3,5-trizaine in CD$_3$CN at 293 K

Figure 7S. $^1$H NMR spectrum of 1,3,5-trizaine in CD$_3$CN at 293 K
Figure 8S. $^1$H NMR spectrum of helicate I with 1,3,5-trimethoxybenzene in CD$_3$CN at 293 K

Figure 9S. $^1$H NMR spectrum of 1,3,5-trimethoxybenzene in CD$_3$CN at 293 K
Figure 10S. $^1$H NMR spectrum of helicate 1 with Triphenylamine in CD$_3$CN at 293 K

Figure 11S. $^1$H NMR spectrum of Triphenylamine in CD$_3$CN at 293 K
Figure 12S. $^1$H NMR spectrum of helicate 1 with pyren-1-ol in CD$_3$CN at 293 K

Figure 13S. $^1$H NMR spectrum of pyren-1-ol in CD$_3$CN at 293 K
Figure 14S. $^1$H NMR spectrum of helicate 1 with 5'-phenyl-1,1':3',1''-terphenyl in CD$_3$CN at 293 K

Figure 15S. $^1$H NMR spectrum of 5'-phenyl-1,1':3',1''-terphenyl in CD$_3$CN at 293 K
UV-Vis SPECTRUMS OF HOST-GUEST INTERACTIONS

Figure 16S. UV–vis spectra of host (helicate 1), guest (pyrene) and the mixture of host and guest

Figure 17S. UV–vis absorption of host-guest complex (helicate 1 + pyrene) compared with observed and calculated value
Figure 18S. UV–vis spectra of host (helicate 1), guest (pyren-1-ol) and the mixture of host and guest.

Figure 19S. UV–vis absorption of host-guest complex (helicate 1 + pyren-1-ol) compared with observed and calculated value.
Figure 20S. Isotope peaks of [Fe₂L₃]^{4+}

Table 1S. Comparison between the calculated and observed intensities of [Fe₂L₃]^{4+} isotope peaks

<table>
<thead>
<tr>
<th>[Fe₂L₃]^{4+} ( [C₉₉H₇₂Fe₂N₂₄]^{4+} ) m/z</th>
<th>426.9</th>
<th>427.1</th>
<th>427.4</th>
<th>427.6</th>
<th>427.9</th>
<th>428.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated relative abundance (%)</td>
<td>12.17</td>
<td>85.33</td>
<td>100</td>
<td>61.21</td>
<td>25.16</td>
<td>7.75</td>
</tr>
<tr>
<td>Observed relative abundance (%)</td>
<td>13.66</td>
<td>91.53</td>
<td>100</td>
<td>60.38</td>
<td>24.52</td>
<td>9.82</td>
</tr>
</tbody>
</table>
**Figure 21S. Isotope peaks of protonated ligand (HL⁺)**

**Table 2S.** Comparison between the calculated and observed intensities of HL⁺ isotope peaks

<table>
<thead>
<tr>
<th>HL⁺ ([C₃₅H₂₅N₈]⁺) m/z</th>
<th>533.2</th>
<th>534.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated relative abundance (%)</td>
<td>100</td>
<td>39.96</td>
</tr>
<tr>
<td>Observed relative abundance (%)</td>
<td>100</td>
<td>36.69</td>
</tr>
</tbody>
</table>
**Figure 22S.** Isotope peaks of $[\text{Fe}_2\text{L}_3(\text{CF}_3\text{SO}_3)]^{3+}$

<table>
<thead>
<tr>
<th>$[\text{Fe}_2\text{L}_3(\text{CF}<em>3\text{SO}<em>3)]^{3+}$ ($[\text{C}</em>{100}\text{H}</em>{72}\text{Fe}<em>2\text{N}</em>{24}\text{O}_3\text{S}]^{+}$)</th>
<th>m/z</th>
<th>618.8</th>
<th>619.1</th>
<th>619.5</th>
<th>619.8</th>
<th>620.1</th>
<th>620.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated relative abundance (%)</td>
<td>12.11</td>
<td>84.12</td>
<td>100</td>
<td>66.01</td>
<td>30.77</td>
<td>1</td>
<td>1.18</td>
</tr>
<tr>
<td>Observed relative abundance (%)</td>
<td>12.80</td>
<td>87.20</td>
<td>100</td>
<td>64.48</td>
<td>30.95</td>
<td>10</td>
<td>52</td>
</tr>
</tbody>
</table>

This is an open-access article distributed under the terms of the Creative Commons Attribution License.