## Supporting Information

**Ag(I)-Catalyzed Cycloisomerization Reactions: Synthesis of Substituted Phenanthrenes and Naphthothiophenes**

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Figure 1. X-Ray Crystallographic Studies. (Thermal ellipsoid are drawn at 30% probability level).

The intensity data for was collected on an Oxford Xcalibur CCD diffractometer equipped with graphite monochromatic Mo-Ka radiation ($\lambda = 0.71073$ Å) at 150(2) K\(^1\). A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on $F^2$ using SHELXL97\(^2\). The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package\(^3\). CCDC deposit no is 884177
### Table 1. Crystal data and structure refinement for 2c.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Empirical formula</strong></td>
<td>C25 H24 O</td>
</tr>
<tr>
<td><strong>Formula weight</strong></td>
<td>340.44</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>150(2) K</td>
</tr>
<tr>
<td><strong>Wavelength</strong></td>
<td>0.71073 Å</td>
</tr>
<tr>
<td><strong>Crystal system</strong></td>
<td>Orthorhombic</td>
</tr>
<tr>
<td><strong>Space group</strong></td>
<td>P b c a</td>
</tr>
<tr>
<td><strong>a</strong></td>
<td>19.703(2) Å</td>
</tr>
<tr>
<td><strong>b</strong></td>
<td>8.2643(5) Å</td>
</tr>
<tr>
<td><strong>c</strong></td>
<td>23.1696(19) Å</td>
</tr>
<tr>
<td><strong>α</strong></td>
<td>90°</td>
</tr>
<tr>
<td><strong>β</strong></td>
<td>90°</td>
</tr>
<tr>
<td><strong>γ</strong></td>
<td>90°</td>
</tr>
<tr>
<td><strong>Volume</strong></td>
<td>3772.7(6) Å</td>
</tr>
<tr>
<td><strong>Z</strong></td>
<td>8</td>
</tr>
<tr>
<td><strong>Density (calculated)</strong></td>
<td>1.199 Mg/m³</td>
</tr>
<tr>
<td><strong>Absorption coefficient</strong></td>
<td>0.071 mm⁻¹</td>
</tr>
<tr>
<td><strong>F(000)</strong></td>
<td>1456</td>
</tr>
<tr>
<td><strong>Crystal size</strong></td>
<td>0.23 x 0.22 x 0.22 mm³</td>
</tr>
<tr>
<td><strong>Theta range for data collection</strong></td>
<td>3.20 to 25.00°.</td>
</tr>
<tr>
<td><strong>Index ranges</strong></td>
<td>-23 ≤ h ≤ 22, -9 ≤ k ≤ 9, -27 ≤ l ≤ 22</td>
</tr>
<tr>
<td><strong>Reflections collected</strong></td>
<td>13457</td>
</tr>
<tr>
<td><strong>Independent reflections</strong></td>
<td>3315 [R(int) = 0.0469]</td>
</tr>
<tr>
<td><strong>Completeness to theta = 25.00°</strong></td>
<td>99.8 %</td>
</tr>
<tr>
<td><strong>Absorption correction</strong></td>
<td>Multi-scan</td>
</tr>
<tr>
<td><strong>Max. and min. Transmission</strong></td>
<td>0.9845 and 0.9838</td>
</tr>
<tr>
<td><strong>Refinement method</strong></td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td><strong>Data / restraints / parameters</strong></td>
<td>3315 / 0 / 235</td>
</tr>
<tr>
<td><strong>Goodness-of-fit on F²</strong></td>
<td>1.096</td>
</tr>
<tr>
<td><strong>Final R indices [I&gt;2sigma(I)]²b</strong></td>
<td>R1 = 0.0969, wR2 = 0.2312</td>
</tr>
<tr>
<td><strong>R indices (all data)</strong></td>
<td>R1 = 0.1223, wR2 = 0.2465</td>
</tr>
<tr>
<td><strong>Largest diff. peak and hole</strong></td>
<td>0.230 and -0.210 e.Å⁻³</td>
</tr>
</tbody>
</table>

\(^a\) R = \(\sum(\|F_o\| - \|F_c\|)/\sum|F_o|\); \(^b\) R_w = ([\sum w(F_o^2 - F_c^2)^2]/[\sum w(F_o^2)])^{1/2}

References:


Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR
$^1$H NMR

Methyl 2'-'((4-ethylphenyl)ethynyl)-[1,1'-biphenyl]-4-carboxylate (1q)
Methyl 2'-(4-ethylphenyl)ethynyl)-[1,1'-biphenyl]-4-carboxylate (1q)
$^1$H NMR

2-Methoxy-10-phenylphenanthrene (2a)
$^{13}$C NMR

2-Methoxy-10-phenylphenanthrene (2a)
$^1$H NMR

2-Methoxy-10-p-tolyl-phenanthrene (2b)
$^{13}$C NMR

2-Methoxy-10-p-tolyl-phenanthrene (2b)
$^1$H NMR

10-[(4-tert-Butyl-phenyl)-2-methoxy-phenanthrene (2c)
$^{13}$C NMR

10-(4-tert-Butyl-phenyl)-2-methoxy-phenanthrene (2c)
$^1$H NMR

2-Methoxy-10-(m-tolyl)phenanthrene (2d)
$^{13}$C NMR

2-Methoxy-10-(m-tolyl)phenanthrene (2d)
$^1$H NMR

10-(4-tert-Butyl-phenyl)-2-methyl-phenanthrene (2e)
$^{13}$C NMR

10-(4-tert-Butyl-phenyl)-2-methyl-phenanthrene (2e)
$^1$H NMR

2-Ethyl-10-(4-ethyl-phenyl)-phenanthrene (2f)
$^{13}$C NMR

2-Ethyl-10-(4-ethyl-phenyl)-phenanthrene (2f)
$^1$H NMR

10-(4-tert-Butyl-phenyl)-2-ethyl-phenanthrene (2g)
$^{13}$C NMR

10-(4-tert-Butyl-phenyl)-2-ethyl-phenanthrene (2g)
$^1$H NMR

2-ethyl-10-(3-methoxyphenyl)phenanthrene (2h)
$^{13}$C NMR

2-ethyl-10-(3-methoxyphenyl)phenanthrene (2h)
$^1$H NMR

2-Isopropoxy-10-phenylphenanthrene (2i)
$^{13}$C NMR

2-Isopropoxy-10-phenylphenanthrene (2i)
$^1$H NMR

10-(4-Ethylphenyl)-2-isopropoxyphenanthrene (2j)
$^{13}$C NMR

10-(4-Ethylphenyl)-2-isopropoxyphenanthrene (2j)
$^1$H NMR

10-(4-tert-Butyl-phenyl)-2-propoxy-phenanthrene (2k)
$^{13}$C NMR

10-(4-tert-Butyl-phenyl)-2-propoxy-phenanthrene (2k)
$^1$H NMR

10-(4-butylphenyl)-1,2-dimethoxyphenanthrene (2l)
$^{13}$C NMR

10-(4-butyphenyl)-1,2-dimethoxyphenanthrene (2l)
$^1$H NMR

1,2-dimethoxy-10-(3-methoxyphenyl)phenanthrene (2m)
$^{13}$C NMR

1,2-dimethoxy-10-(3-methoxyphenyl)phenanthrene (2m)
$^1$H NMR

2-(4-Fluoro-phenoxymethyl)-10-p-tolyl-phenanthrene (2n)
$^{13}$C NMR

2-(4-Fluoro-phenoxy)methyl)-10-$p$-tolyl-phenanthrene (2n)
$^1$H NMR

10-(4-Ethylphenyl)-2-(phenoxyethyl)phenanthrene (2o)
$^{13}$C NMR

10-(4-Ethylphenyl)-2-(phenoxy methyl)phenanthrene (2o)
$^1$H NMR

10-(4-Ethylphenyl)-4-phenylphenanthrene (2p)

[Chemical Structure Image]

[1H NMR Spectrum Image]
$^{13}$C NMR

10-(4-Ethylphenyl)-4-phenylphenanthrene (2p)
$^1$H NMR

5-(4-Methoxyphenyl)-7-methylnaphtho[1,2-b]thiophene (4a)
$^{13}$C NMR

5-(4-Methoxyphenyl)-7-methylnaphtho[1,2-\textit{b}]thiophene (4a)
$^1$H NMR

5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[1,2-$b$]thiophene (4b)
$^{13}$C NMR

5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[1,2-b]thiophene (4b)
$^1$H NMR

7-Ethyl-5-(4-methoxyphenyl)naphtho[1,2-b]thiophene (4c)
$^{13}$C NMR

$7$-Ethyl-5-(4-methoxyphenyl)naphtho[1,2-$b$]thiophene (4c)
$^1$H NMR

7-Ethyl-5-(p-tolyl)naphtho[1,2-\(b\)]thiophene (4d)
$^{13}$C NMR

7-Ethyl-5-(p-tolyl)naphtho[1,2-\(b\)]thiophene (4d)
$^{1}H$ NMR

7-Fluoro-5-(4-methoxyphenyl)naphtho[1,2-b]thiophene (4e)
$^{13}$C NMR

7-Fluoro-5-(4-methoxyphenyl)naphtho[1,2-b]thiophene (4e)
$^1$H NMR

5-(4-Ethylphenyl)-7-methylnaptho[2,1-b]thiophene (6a)
$^{13}$C NMR

5-(4-Ethylphenyl)-7-methylnaphtho[2,1-b]thiophene (6a)
$^1$H NMR

5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[2,1-b]thiophene (6b)
$^{13}$C NMR

5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[2,1-b]thiophene (6b)
$^1$H NMR

7-Ethyl-5-phenylnaphtho[2,1-b]thiophene (6c)
$^{13}$C NMR

7-Ethyl-5-phenynaphtho[2,1-$b$]thiophene (6c)
$^1$H NMR

7-Methoxy-5-(p-tolyl)naphtho[2,1-b]thiophene (6d)
$^{13}$C NMR

7-Methoxy-5-(p-tolyl)naphtho[2,1-b]thiophene (6d)
$^1$H NMR

5,9-Diphenylnaptho[2,1-b]thiophene (6e)
$^{13}$C NMR

5,9-Diphenyl[naphtho[2,1-b]thiophene (6e)