Supporting Information

Metal Triflates Promoted Synthesis of Naphthalenes

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(1) Additional scanned photocopies (pages S-2~S-27)
(2) X-ray crystal data of 5e, 5f, 8d, 8g, 9a and 9b (pages S-28~S-33)
Compound 5a
Compound 5h
Compound 5i
Compound 5j
Compound 5k
Compound 5m
Compound 5n
Compound 7b
Compound 8b
Compound 8c
Compound 8d
Compound 8e
Compound 8f
Compound 8g
Compound 9a
### X-ray crystal data of 5e

![Chemical structure of 5e](image)

**Empirical formula**: C17 H14 O2  
**Formula weight**: 250.28  
**Temperature**: 100(2) K  
**Wavelength**: 0.71073 Å  
**Crystal system**: Orthorhombic  
**Space group**: F d d 2  
**Unit cell dimensions**:  
- \(a = 13.3885(3) \text{ Å} \)  
- \(b = 66.3135(18) \text{ Å} \)  
- \(c = 5.5816(2) \text{ Å} \)  
**Volume**: 4955.6(2) Å³  
**Z**: 16  
**Density (calculated)**: 1.342 Mg/m³  
**Absorption coefficient**: 0.087 mm⁻¹  
**F(000)**: 2112  
**Crystal size**: 0.25 x 0.25 x 0.12 mm³  
**Theta range for data collection**: 1.23 to 26.39°.  
**Index ranges**: -10<=h<=16, -82<=k<=82, -6<=l<=6  
**Reflections collected**: 11029  
**Independent reflections**: 2518 \([R(int) = 0.0603]\)  
**Completeness to theta = 26.39°**: 99.9 %  
**Absorption correction**: Semi-empirical from equivalents  
**Max. and min. transmission**: 0.9486 and 0.8690  
**Refinement method**: Full-matrix least-squares on F²  
**Data / restraints / parameters**: 2518 / 1 / 174  
**Goodness-of-fit on F²**: 1.168  
**Final R indices [I>2sigma(I)]**: R1 = 0.0325, wR2 = 0.0807  
**R indices (all data)**: R1 = 0.0428, wR2 = 0.1154  
**Absolute structure parameter**: 0.2(13)  
**Largest diff. peak and hole**: 0.404 and -0.542 e.Å⁻³
X-ray crystal data of 5f

Empirical formula: C17 H13 F O2

Formula weight: 268.27

Temperature: 100(2) K

Wavelength: 0.71073 Å

Crystal system: Triclinic

Space group: P -1

Unit cell dimensions:
- a = 6.7021(11) Å, α = 85.327(6)°.
- b = 7.9371(12) Å, β = 80.530(6)°.
- c = 12.170(2) Å, γ = 82.517(6)°.

Volume: 631.92(18) Å³

Z: 2

Density (calculated): 1.410 Mg/m³

Absorption coefficient: 0.101 mm⁻¹

F(000): 280

Crystal size: 0.18 x 0.10 x 0.10 mm³

Theta range for data collection: 1.70 to 26.38°.

Index ranges:
- -8 <= h <= 7,
- -9 <= k <= 7,
- -15 <= l <= 15

Reflections collected: 9259

Independent reflections: 2547 [R(int) = 0.0243]

Completeness to theta = 26.38°: 98.6 %

Absorption correction: Semi-empirical from equivalents

Max. and min. transmission: 0.9486 and 0.9019

Refinement method: Full-matrix least-squares on F²

Data / restraints / parameters: 2547 / 0 / 183

Goodness-of-fit on F²: 1.089

Final R indices [I>2sigma(I)]: R1 = 0.0343, wR2 = 0.0907

R indices (all data): R1 = 0.0431, wR2 = 0.1097

Largest diff. peak and hole: 0.231 and -0.223 e.Å⁻³
X-ray crystal data of 8d

Empirical formula
C19 H18 O3

Formula weight
294.33

Temperature
100(2) K

Wavelength
0.71073 Å

Crystal system
Monoclinic

Space group
P 21/c

Unit cell dimensions
\(a = 13.3450(12) \text{ Å} \quad \alpha = 90^\circ\).
\(b = 15.2538(14) \text{ Å} \quad \beta = 99.819(2)^\circ\).
\(c = 7.5723(7) \text{ Å} \quad \gamma = 90^\circ\).

Volume
1518.9(2) Å³

Z
4

Density (calculated)
1.287 Mg/m³

Absorption coefficient
0.086 mm⁻¹

F(000)
624

Crystal size
0.15 x 0.10 x 0.10 mm³

Theta range for data collection
2.045 to 26.421°.

Index ranges
\(-16 \leq h \leq 16, -18 \leq k \leq 19, -9 \leq l \leq 4\)

Reflections collected
12198

Independent reflections
3116 [R(int) = 0.0580]

Completeness to theta = 25.242°
100.0 %

Absorption correction
Semi-empirical from equivalents

Max. and min. transmission
0.9485 and 0.8689

Refinement method
Full-matrix least-squares on F²

Data / restraints / parameters
3116 / 0 / 202

Goodness-of-fit on F²
0.996

Final R indices [I>2sigma(I)]
R1 = 0.0504, wR2 = 0.1026

R indices (all data)
R1 = 0.1172, wR2 = 0.1285

Extinction coefficient
n/a

Largest diff. peak and hole
0.146 and -0.186 e.Å⁻³
X-ray crystal data of 8g

Empirical formula: C_{24}H_{20}O_{2}

Formula weight: 340.40

Temperature: 100(2) K

Wavelength: 0.71073 Å

Crystal system: Triclinic

Space group: P -1

Unit cell dimensions:
- \( a = 6.6111(3) \, \text{Å} \)  
- \( \alpha = 106.574(2)^\circ \)
- \( b = 9.8830(5) \, \text{Å} \)  
- \( \beta = 94.682(2)^\circ \)
- \( c = 14.4700(8) \, \text{Å} \)  
- \( \gamma = 104.105(2)^\circ \)

Volume: 867.14(8) Å\(^3\)

Z: 2

Density (calculated): 1.304 Mg/m\(^3\)

Absorption coefficient: 0.082 mm\(^{-1}\)

F(000): 360

Crystal size: 0.12 x 0.10 x 0.10 mm\(^3\)

Theta range for data collection: 1.488 to 26.356\(^\circ\)

Index ranges:
- \(-7 < h < 8\)
- \(-12 < k < 10\)
- \(-17 < l < 18\)

Reflections collected: 11883

Independent reflections: 3534 \([R(int) = 0.0262]\)

Completeness to theta = 25.242\(^\circ\): 99.7 %

Absorption correction: Semi-empirical from equivalents

Max. and min. transmission: 0.9485 and 0.8919

Refinement method: Full-matrix least-squares on \( F^2 \)

Data / restraints / parameters: 3534 / 0 / 237

Goodness-of-fit on \( F^2 \): 1.072

Final R indices \([I>2\sigma(I)]\):
- \( R1 = 0.0386 \)
- \( wR2 = 0.1084 \)

R indices (all data):
- \( R1 = 0.0460 \)
- \( wR2 = 0.1231 \)

Extinction coefficient: n/a

Largest diff. peak and hole: 0.231 and -0.211 e.Å\(^{-3}\)

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**X-ray crystal data of 9a**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C18 H16 O2</td>
</tr>
<tr>
<td>Formula weight</td>
<td>264.31</td>
</tr>
<tr>
<td>Temperature</td>
<td>295(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>P 1 21/c 1</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a = 7.654(4) Å, α = 90°</td>
</tr>
<tr>
<td></td>
<td>b = 13.820(8) Å, β = 98.379(9)°</td>
</tr>
<tr>
<td></td>
<td>c = 13.657(8) Å, γ = 90°</td>
</tr>
<tr>
<td>Volume</td>
<td>1429.0(14) Å³</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>1.229 Mg/m³</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>0.079 mm⁻¹</td>
</tr>
<tr>
<td>F(000)</td>
<td>560</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.30 x 0.20 x 0.18 mm³</td>
</tr>
<tr>
<td>Theta range for data collection</td>
<td>2.11 to 26.46°</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-9 &lt;= h &lt;= 9, -17 &lt;= k &lt;= 15, -12 &lt;= l &lt;= 17</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>8979</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>2937 [R(int) = 0.0271]</td>
</tr>
<tr>
<td>Completeness to theta = 26.46°</td>
<td>99.4 %</td>
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<tr>
<td>Absorption correction</td>
<td>Semi-empirical from equivalents</td>
</tr>
<tr>
<td>Max. and min. transmission</td>
<td>0.9486 and 0.8266</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
<td>2937 / 0 / 183</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.049</td>
</tr>
<tr>
<td>Final R indices [I&gt;2sigma(I)]</td>
<td>R1 = 0.0475, wR2 = 0.1271</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>R1 = 0.0711, wR2 = 0.1581</td>
</tr>
<tr>
<td>Largest diff. peak and hole</td>
<td>0.160 and -0.175 e Å⁻³</td>
</tr>
</tbody>
</table>
X-ray crystal data of 9b

Empirical formula: C19 H18 O3

Formula weight: 294.33

Temperature: 100(2) K

Wavelength: 0.71073 Å

Crystal system: Monoclinic

Space group: C 1 c 1

Unit cell dimensions:
- a = 8.6905(3) Å, α = 90°
- b = 21.9250(7) Å, β = 108.3260(10)°
- c = 8.2652(3) Å, γ = 90°

Volume: 1494.97(9) Å³

Z: 4

Density (calculated): 1.308 Mg/m³

Absorption coefficient: 0.088 mm⁻¹

F(000): 624

Crystal size: 0.30 x 0.25 x 0.25 mm³

Theta range for data collection: 1.86 to 26.52°

Index ranges:
- -8 ≤ h ≤ 10
- -27 ≤ k ≤ 27
- -10 ≤ l ≤ 10

Reflections collected: 5988

Independent reflections: 2742 [R(int) = 0.0146]

Completeness to theta = 26.52°: 99.0%

Absorption correction: Semi-empirical from equivalents

Max. and min. transmission: 0.9486 and 0.8716

Refinement method: Full-matrix least-squares on F²

Data / restraints / parameters: 2742 / 2 / 202

Goodness-of-fit on F²: 1.052

Final R indices [I>2sigma(I)]:
- R1 = 0.0277, wR2 = 0.0732

R indices (all data):
- R1 = 0.0291, wR2 = 0.0743

Absolute structure parameter: 0.9(7)

Largest diff. peak and hole: 0.194 and -0.156 e.Å⁻³