Supporting Information

Pd(OAc)$_2$-Mediated Dimerization/Cycloisomerization of 2-Sulfonyl-4-alkynones: Synthesis of trans-1,2-Difurylethlenes

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Compound 5a (1H-NMR spectral data)
Compound 5a ($^{13}$C-NMR spectral data)
Compound 5a-1 (1H-NMR spectral data)
Compound 5a-1 (\(^1\)H-NMR spectral data)
Compound 5b (¹H-NMR spectral data)
Compound 5b (\(^{13}\text{C})-\text{NMR spectral data} \)
Compound 5c (¹H-NMR spectral data)
Compound 5c ($^{13}$C-NMR spectral data)
Compound 5d (¹H-NMR spectral data)
Compound 5d (¹³C-NMR spectral data)
Compound 5e (\textsuperscript{1}H-NMR spectral data)
Compound 5e ($^{13}$C-NMR spectral data)
Compound 5f (\(^1\)H-NMR spectral data)
Compound 5f \(^{13}\text{C}-\text{NMR spectral data}\)
Compound 5g (\(^1\)H-NMR spectral data)
Compound 5g ($^{13}$C-NMR spectral data)
Compound 5h (¹H-NMR spectral data)
Compound 5h (13C-NMR spectral data)
Compound 5i (1H-NMR spectral data)
Compound 5i ($^{13}$C-NMR spectral data)
Compound 5j (\(^1\)H-NMR spectral data)
Compound 5j \(^{13}\text{C}-\text{NMR spectral data}\)
Compound 5k (\(^1\)H-NMR spectral data)
Compound 5k (\(^{13}\)C-NMR spectral data)
Compound 5l (¹H-NMR spectral data)
Compound 5l ($^{13}$C-NMR spectral data)

Pulse Sequence: s2pu1
UNITYplus-400 =unity400"
Date: Oct 19 2018
Solvent: CDCl3
Ambient temperature
Total 4000 repetitions

[Chemical structure image]

[Graph showing NMR spectral data]

S-27
Compound 5m (\(^1\)H-NMR spectral data)

KSY16FF
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Sep 27 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

\[
\begin{align*}
\text{Me} & \quad \text{Me} \\
\text{O} & \quad \text{O} \\
\text{Me} & \quad \text{Me} \\
\text{Me} & \quad \text{Me}
\end{align*}
\]
Compound 5m ($^{13}$C-NMR spectral data)
Compound 5n (\textsuperscript{1}H-NMR spectral data)
Compound 5n ($^{13}$C-NMR spectral data)
Compound 5o ('H-NMR spectral data)
Compound 5o (\textsuperscript{13}C-NMR spectral data)
Compound 5p (¹H-NMR spectral data)
Compound 5p ($^{13}$C-NMR spectral data)
Compound 5q ($^{13}$C-NMR spectral data)
Compound 5r (1H-NMR spectral data)
Compound 5r ($^{13}$C-NMR spectral data)
Compound 5s (¹H-NMR spectral data)
Compound 5s ($^{13}$C-NMR spectral data)
Compound 5t (¹H-NMR spectral data)
Compound 5t ($^{13}$C-NMR spectral data)
Compound 5u (\(^1\)H-NMR spectral data)
Compound 5u (\(^{13}\text{C}-\text{NMR spectral data})
Compound 6a (¹H-NMR spectral data)
Compound 6a ($^{13}$C-NMR spectral data)
Compound 6b (\(^1\)H-NMR spectral data)
Compound 6b ($^{13}$C-NMR spectral data)
X-ray crystal data of compound 5h

Empirical formula  
C36 H28 O8 S2

Formula weight  
652.70

Temperature  
99(2) K

Wavelength  
0.71073 Å

Crystal system  
Triclinic

Space group  
P -1

Unit cell dimensions  

\[ a = 6.1107(2) \text{ Å} \quad \alpha = 92.857(2)^\circ. \]
\[ b = 8.2434(3) \text{ Å} \quad \beta = 94.178(2)^\circ. \]
\[ c = 14.5419(5) \text{ Å} \quad \gamma = 91.223(2)^\circ. \]

Volume  
729.43(4) Å³

Z  
1

Density (calculated)  
1.486 Mg/m³

Absorption coefficient  
0.241 mm⁻¹

F(000)  
340

Crystal size  
0.20 x 0.15 x 0.04 mm³

Theta range for data collection  

Index ranges  

\[-7 \leq h \leq 7, \quad -10 \leq k \leq 10, \quad -18 \leq l \leq 18\]

Reflections collected  
14412

Independent reflections  
2997 [R(int) = 0.0271]

Completeness to theta = 25.242°  
99.7 %

Absorption correction  
Semi-empirical from equivalents

Max. and min. transmission  
0.7454 and 0.7121

Refinement method  
Full-matrix least-squares on F²

Data / restraints / parameters  
2997 / 0 / 209

Goodness-of-fit on F²  
1.051

Final R indices [I>2sigma(I)]  
R1 = 0.0387, wR2 = 0.0988

R indices (all data)  
R1 = 0.0445, wR2 = 0.1027

Extinction coefficient  
na

Largest diff. peak and hole  
0.717 and -0.377 e.Å⁻³
The thermal ellipsoid was drawn at the 50% probability level.
X-ray crystal data of compound 5r

Empirical formula C18 H14 O3 S
Formula weight 310.35
Temperature 100(2) K
Wavelength 0.71073 Å
Crystal system Monoclinic
Space group P 21/c
Unit cell dimensions
  a = 8.2977(4) Å  α = 90°.
  b = 21.6906(9) Å  β = 91.674(2)°.
  c = 8.2477(4) Å  γ = 90°.
Volume 1483.80(12) Å³
Z 4
Density (calculated) 1.389 Mg/m³
Absorption coefficient 0.228 mm⁻¹
F(000) 648
Crystal size 0.20 x 0.18 x 0.18 mm³
Theta range for data collection 1.878 to 26.402°.
Index ranges -10<=h<=10, -27<=k<=27, -10<=l<=10
Reflections collected 19288
Independent reflections 3046 [R(int) = 0.0329]
Completeness to theta = 25.242° 99.9 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7454 and 0.7033
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 3046 / 0 / 200
Goodness-of-fit on F² 1.074
Final R indices [I>2sigma(I)] R1 = 0.0361, wR2 = 0.0947
R indices (all data) R1 = 0.0426, wR2 = 0.1045
Extinction coefficient n/a
Largest diff. peak and hole 0.453 and -0.429 e.Å⁻³
The thermal ellipsoid was drawn at the 50% probability level.
### X-ray crystal data of compound 6b

![Structural formula of compound 6b]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Empirical formula C22 H18 O2</td>
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<tr>
<td>Formula weight 157.18</td>
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<tr>
<td>Temperature 100(2) K</td>
<td></td>
</tr>
<tr>
<td>Wavelength 0.71073 Å</td>
<td></td>
</tr>
<tr>
<td>Crystal system Monoclinic</td>
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</tr>
<tr>
<td>Space group P 21/c</td>
<td></td>
</tr>
<tr>
<td>Unit cell dimensions</td>
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</tr>
<tr>
<td>a = 5.4702(2) Å, α = 90°</td>
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</tr>
<tr>
<td>b = 20.9156(8) Å, β = 102.371(2)°</td>
<td></td>
</tr>
<tr>
<td>c = 7.4643(3) Å, γ = 90°</td>
<td></td>
</tr>
<tr>
<td>Volume 834.18(6) Å^3</td>
<td></td>
</tr>
<tr>
<td>Z 4</td>
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<tr>
<td>Density (calculated) 1.252 Mg/m^3</td>
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<tr>
<td>Absorption coefficient 0.079 mm^-1</td>
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<tr>
<td>F(000) 332</td>
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<tr>
<td>Crystal size 0.10 x 0.02 x 0.01 mm^3</td>
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<td>Theta range for data collection 1.947 to 26.401°</td>
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<tr>
<td>Index ranges -4&lt;=h&lt;=6, -25&lt;=k&lt;=26, -9&lt;=l&lt;=9</td>
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<tr>
<td>Reflections collected 6287</td>
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<tr>
<td>Independent reflections 1712 [R(int) = 0.0264]</td>
<td></td>
</tr>
<tr>
<td>Completeness to theta = 25.242° 99.8 %</td>
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<tr>
<td>Absorption correction Semi-empirical from equivalents</td>
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<tr>
<td>Max. and min. transmission 0.7454 and 0.6913</td>
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<tr>
<td>Refinement method Full-matrix least-squares on F^2</td>
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</tr>
<tr>
<td>Data / restraints / parameters 1712 / 0 / 109</td>
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<tr>
<td>Goodness-of-fit on F^2 1.053</td>
<td></td>
</tr>
<tr>
<td>Final R indices [I&gt;2sigma(I)] R1 = 0.0383, wR2 = 0.0874</td>
<td></td>
</tr>
<tr>
<td>R indices (all data) R1 = 0.0535, wR2 = 0.0950</td>
<td></td>
</tr>
<tr>
<td>Extinction coefficient n/a</td>
<td></td>
</tr>
<tr>
<td>Largest diff. peak and hole 0.215 and -0.226 e.Å^-3</td>
<td></td>
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</tbody>
</table>
The thermal ellipsoid was drawn at the 50% probability level.