Supplementary Material

Samarium triflate-catalyzed dimerization of vinylarenes

Meng-Yang Chang*\textsuperscript{a,b} and Yu-Lin Tsai\textsuperscript{a}
\textsuperscript{a} Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 807, Taiwan
\textsuperscript{b} Department of Medical Research, Kaohsiung Medical University Hospital, Kaohsiung 807, Taiwan
Email: mychang@kmu.edu.tw

Table of Contents

$^1$H NMR and $^{13}$C NMR spectra copies of compounds 4\textit{a}, 4\textit{c}-\textit{n}, 4\textit{q}, 4\textit{b}-\textit{1}, 4\textit{e}-\textit{1}, 4\textit{f}-\textit{1}, 4\textit{g}-\textit{1}, 4\textit{o}-\textit{1} and 4\textit{p}-\textit{1}........S2
X-ray crystal data of compound 4\textit{k}......................................................................................................................S22
Compound 4a
Compound 4b-1
Compound 4c
Compound 4d
Compound 4e
Compound 4e-1
Compound 4f
Compound 4f-1
Compound 4g
Compound 4g-1
Compound 4h
Compound 4i
Compound 4j
Compound 4k
Compound 4l
Compound 4m
Compound 4n
Compound 4o-1
Compound 4p-1
Compound 4q
X-ray crystal data of compound 4k

Empirical formula: C50 H64 O8
Formula weight: 793.01
Temperature: 100(2) K
Wavelength: 0.71073 Å
Crystal system: Triclinic
Space group: P -1
Unit cell dimensions:
- a = 9.4024(3) Å  \( \alpha = 98.783(2)^\circ \)
- b = 15.5199(5) Å  \( \beta = 105.756(2)^\circ \)
- c = 16.4035(6) Å  \( \gamma = 104.7270(10)^\circ \)
Volume: 2163.91(13) Å³
Z: 2
Density (calculated): 1.217 Mg/m³
Absorption coefficient: 0.081 mm⁻¹
F(000): 856
Crystal size: 0.18 x 0.15 x 0.05 mm³
Theta range for data collection: 1.328 to 26.411°.
Index ranges: -11<=h<=11, -19<=k<=19, -20<=l<=20
Reflections collected: 31205
Independent reflections: 8872 [R(int) = 0.0374]
Completeness to theta = 25.242°: 99.8 %
Absorption correction: Semi-empirical from equivalents
Max. and min. transmission: 0.9485 and 0.9042
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 8872 / 0 / 539
Goodness-of-fit on F²: 1.059
Final R indices [I>2sigma(I)]: R1 = 0.0771, wR2 = 0.1993
R indices (all data): R1 = 0.0976, wR2 = 0.2137
Extinction coefficient: n/a
Largest diff. peak and hole: 1.290 and -0.428 e.Å⁻³
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180413LT_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: 180413LT_0m**

<table>
<thead>
<tr>
<th>Bond precision: C-C = 0.0042 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td></td>
</tr>
<tr>
<td>a = 9.4024(3)</td>
<td>b = 15.5199(5)</td>
</tr>
<tr>
<td>alpha = 98.783(2)</td>
<td>beta = 105.756(2)</td>
</tr>
<tr>
<td>c = 16.4035(6)</td>
<td>gamma = 104.727(1)</td>
</tr>
<tr>
<td>Temperature: 100 K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>2163.92(13)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C25 H32 O4</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C25 H32 O4</td>
</tr>
<tr>
<td>Mr</td>
<td>396.51</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.217</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.081</td>
</tr>
<tr>
<td>F000</td>
<td>856.0</td>
</tr>
<tr>
<td>F000’</td>
<td>856.40</td>
</tr>
<tr>
<td>h,k,l_max</td>
<td>11,19,20</td>
</tr>
<tr>
<td>Nref</td>
<td>8898</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.986, 0.996</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.986</td>
</tr>
</tbody>
</table>

Correction method = # Reported T Limits: Tmin=0.904 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness = 0.997 θ(max) = 26.411

R(reflections) = 0.0771(6827) wR2(reflections) = 0.2137(8872)

S = 1.059 Npar = 539

The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.
The thermal ellipsoid was drawn at the 50% probability level.