Supplementary Material

Samarium triflate-catalyzed dimerization of vinylarenes

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Compound 4b-1
Compound 4e
Compound 4e-1
Compound 4f
Compound 4f-1
Compound 4g
Compound 4g-1
Compound 4h
Compound 4i
Compound 4j
Compound 4k

[Chemical structure images]

[Chemical spectra images]
Compound 4l
Compound 4m
Compound 4n
Compound 4o-1

[Image of a chemical structure and NMR spectra]

[Additional chemical structure and NMR spectra]
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:

\[
a = 9.4024(3) \, \text{Å} \quad \alpha = 98.783(2)^\circ.
\]
\[
b = 15.5199(5) \, \text{Å} \quad \beta = 105.756(2)^\circ.
\]
\[
c = 16.4035(6) \, \text{Å} \quad \gamma = 104.7270(10)^\circ.
\]
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:

\[-11 \leq h \leq 11, \quad -19 \leq k \leq 19, \quad -20 \leq l \leq 20\]
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**

Bond precision: C-C = 0.0042 Å  Wavelength=0.71073

| Cell:     | a=9.4024(3) | b=15.5199(5) | c=16.4035(6) |
|          | alpha=98.783(2) | beta=105.756(2) | gamma=104.727(1) |
| Temperature: | 100 K |

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</table>

Correction method= # Reported T Limits: Tmin=0.904 Tmax=0.948

AbsCorr = MULTI-SCAN

Data completeness= 0.997  Theta(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