Phosphine-Catalyzed Dearomative (3+2) Annulation of 2-Nitrobenzofurans and Nitrobenzothiophenes with Allenoate

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Supporting Information

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1. X-ray crystal structure of compound 3o

ORTEP of 3o (at 50% level)

Crystal data and structure refinement for 3o (CCDC-1900800)

Identification code 3o
Empirical formula C₁₅H₁₅NO₆
Formula weight 305.28
Temperature/K 293(2)
Crystal system triclinic
Space group P-1
a/Å 6.9301(3)
b/Å 12.5301(7)
c/Å 17.0571(10)
α/° 85.888(5)
β/° 88.194(4)
γ/° 79.004(4)
Volume/Å³ 1449.97(14)
Z 4
ρ_calc/g/cm³ 1.398
μ/mm⁻¹ 0.926
F(000) 640.0
Crystal size/mm³ 0.2 × 0.14 × 0.1
Radiation CuKα (λ = 1.54184)
2Θ range for data collection/° 7.204 to 134.152
Index ranges -8 ≤ h ≤ 5, -14 ≤ k ≤ 14, -20 ≤ l ≤ 20
Reflections collected 10304
Independent reflections 5176 [R_int = 0.0235, R(sigma) = 0.0373]
Data/restraints/parameters 5176/4/418
Goodness-of-fit on F² 1.039
Final R indexes [I>2σ(I)] R₁ = 0.0496, wR₂ = 0.1333
Final R indexes [all data] R₁ = 0.0633, wR₂ = 0.1480
Largest diff. peak/hole / e Å⁻³ 0.20/-0.20
2. $^1$H and $^{13}$C for new substrates 4 and 6

$^1$H and $^{13}$C NMR of 4b
$^1$H and $^{13}$C NMR of 4c
$^1$H and $^{13}$C NMR of 4d
$^1$H and $^{13}$C NMR of 6b
$^{1}H$ and $^{13}C$ NMR of 6c
$^1$H and $^{13}$C NMR of 6d
$^1$H and $^{13}$C NMR of 6e
$^1$H and $^{13}$C NMR of 6f
3. $^1$H and $^{13}$C for compounds 3, 5, 7 and 8

$^1$H and $^{13}$C NMR of 3a
$^1$H and $^{13}$C NMR of 3b
$^1$H and $^{13}$C NMR of 3c
$^1$H and $^{13}$C NMR of 3d
$^1$H and $^{13}$C NMR of 3e
$^1$H and $^{13}$C NMR of 3f
$^1$H and $^{13}$C NMR of 3g
$^1$H and $^{13}$C NMR of 3h
$^1$H and $^{13}$C NMR of 3i
$^1$H and $^{13}$C NMR of 3j
$^1$H and $^{13}$C NMR of 3k
\(^1\text{H}\) and \(^{13}\text{C}\) NMR of 3l
$^1$H and $^{13}$C NMR of 3m
$^1$H and $^{13}$C NMR of 3n
$^1$H and $^{13}$C NMR of 3o
$^1$H and $^{13}$C NMR of $3p$
$^1$H and $^{13}$C NMR of 3q
$^1$H and $^{13}$C NMR of 3r
$^1$H and $^{13}$C NMR of 3s
$^1$H and $^{13}$C NMR of 3t
$^1$H and $^{13}$C NMR of 5a
$^1$H and $^{13}$C NMR of 5b
$^1$H and $^{13}$C NMR of 5c
$^1$H and $^{13}$C NMR of 5d
$^{1}H$ and $^{13}C$ NMR of 5e
$^1$H and $^{13}$C NMR of 7a
$^1$H and $^{13}$C NMR of 7b
$^1$H and $^{13}$C NMR of 7c
$^1$H and $^{13}$C NMR of 7d
$^{1}$H and $^{13}$C NMR of 7e
$^1$H and $^{13}$C NMR of 7f
$^1$H and $^{13}$C NMR of 7g
$^1$H and $^{13}$C NMR of 7h
$^1{\text{H}}$ and $^{13}{\text{C}}$ NMR of 8
$^{1}H$ and $^{13}C$ NMR of 9
HPLC of 3a

### Detector A (254nm)

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**Totals**

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**Totals**

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