# Palladium Catalyzed Synthesis of Poly-substituted and Poly-functionalised <br> <br> Conjugated 1,3-Dienes from Allyl Bromides and $\alpha$-Diazoesters. 

 <br> <br> Conjugated 1,3-Dienes from Allyl Bromides and $\alpha$-Diazoesters.}

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Table of contents

| X-Ray Crystallographic Data for 3a | 3 |
| :--- | :---: |
| ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ spectra | $3-29$ |

## X-Ray Crystallographic Data for 3a:

The structure of 3a was also determined by x-ray analysis. The single crystal for the analysis was grown by slow evaporation of solution of $\mathbf{3 a}$ in hexane-ethylacetate mixture. X Ray Crystallography: CCDC2149586 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

## Crystal data and structure refinement Compound 3a

Formula: $\mathrm{C}_{20} \mathrm{H}_{18} \mathrm{O}_{4}$
Formula weight: $322.34 \mathrm{~g} / \mathrm{mol}$
Wave length: $=0.71073 \AA$
Crystal system: triclinic
Space group: P-1
Color of crystal: colourless
Unit cell parameters: $\mathrm{a}=9.8517(5) \AA \quad \alpha=86.084(2)^{\circ}$

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\begin{array}{ll}
\mathrm{b}=10.0871(5) \AA & \beta=71.973(2)^{\circ} \\
\mathrm{c}=10.0861(5) \AA & \gamma=64.392(2)^{\circ}
\end{array}
$$

Temperature of data collection: 300(2) K
Values of Z, R, GOF:

$$
\begin{aligned}
& \mathrm{Z}=2 \\
& \mathrm{R} \text { (reflections) }=0.0443(2849), \quad \text { wR2(reflections) }=0.1151(3478) \\
& \text { GOF }=1.035
\end{aligned}
$$

Measurement device type: Bruker D8 goniometer
Computing structure solution: SHELXT 2018/2 (Sheldrick, 2018)
Computing structure refinement: SHELXL-2018/3 (Sheldrick, 2018)

${ }^{1} \mathrm{H}-\mathrm{NMR} \mathrm{MHz} \mathrm{of} 3 \mathrm{~b}$.
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum of 3 b .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 c .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 c .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$


$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 d . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum of 3 d .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$


$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 30 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$

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${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 e .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$




${ }^{13} \mathrm{C}$-NMR spectrum of 3 e . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 30 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 f .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 ff . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$



${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 g . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 g . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$


$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 h ． $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum of 3 h ．
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 i .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$



${ }^{13} \mathrm{C}$-NMR spectrum of 3 i . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$

${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 j . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 j .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$


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${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 k .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 k .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 30 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 I .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 I.
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$





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${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 3 m . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 3 m . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 a . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 4 a .

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}$-NMR spectrum of 4 b . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$



${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 c . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 4 c . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$


$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 d . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 4 d .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$


$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 e .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$



$\begin{array}{llllllll}1.5 & 10.5 & 10.0 & 9.5 & 9.0 & 8.5 & 8.0\end{array}$

${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum of 4 e . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 f .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$



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${ }^{13} \mathrm{C}$-NMR spectrum of 4 f . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 g . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum of 4 g . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 80 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 h . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 4 h . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 i . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 4 i . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}10 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$

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${ }^{1} \mathrm{H}$-NMR spectrum of 4 j . $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 4 j . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$

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${ }^{1} \mathrm{H}$-NMR spectrum of 4 k .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum of 4 k .
$100 \mathrm{MHz}, \mathrm{CDCl}_{3}$



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${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 I .
$400 \mathrm{MHz}, \mathrm{CDCl}_{3}$


${ }^{13} \mathrm{C}$-NMR spectrum of 41 . $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$

$\begin{array}{lllllllllllllllllllllll}210 & 200 & 190 & 180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100 & 90 & 50 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0 & -10\end{array}$
${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of 4 m $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$



$\begin{array}{llllllllllllllllllllllllllllllllllll}12.0 & 11.5 & 11.0 & 10.5 & 10.0 & 9.5 & 9.0 & 8.5 & 8.0 & 7.5 & 7.0 & 6.5 & 6.0 & 5.5 & 5.0 & 4.5 & 4.0 & 3.5 & 3.0 & 2.5 & 2.0 & 1.5 & 1.0 & 0.5 & 0.0\end{array}$


