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Correction: C–H nickellation of phenol-derived phosphinites: regioselectivity and structures of cyclonickellated complexes

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Correction for 'C–H nickellation of phenol-derived phosphinites: regioselectivity and structures of cyclonickellated complexes' by Loïc P. Mangin *et al.*, *Dalton Trans.*, 2017, **46**, 16159–16170, DOI: 10.1039/C7DT03403B.

We have noticed that the following incorrectly assigned NMR data need correcting:

1. In the NMR data given for compound **1e**, the assignments of C₃Ar–H and C₄Ar–H should be switched. This assignment was not discussed in the main body of the report, and so a correction of only the data given in the Experimental section is sufficient.

The ¹H NMR and ¹³C data for compound **1e**, given in the left column of page 16168, should be changed as follows:

Incorrectly assigned ¹H NMR data for **1e**
6.70 (ddd, 1H, C₃Ar–H, ³J_{HH} = 8.0, ⁴J_{HP} = 2.1, ⁵J_{HH} = 1.0)
7.12 (dd, 1H, C₄Ar–H, ³J_{HH} = 8.0, ⁵J_{HP} = 1.0)

Corrected assignments for ¹H NMR data for **1e**
6.70 (ddd, 1H, C₄Ar–H, ³J_{HH} = 8.0, ⁴J_{HH} = 2.1, ⁵J_{HP} = 1.0)
7.12 (dd, 1H, C₃Ar–H, ³J_{HH} = 8.0, ⁴J_{HP} = 1.0)

Incorrectly assigned ¹³C NMR data for **1e**
120.66 (d, 1C, C₃Ar–H, ³J_{CP} = 1.6)
139.43 (d, 1C, C₄Ar–H, ⁴J_{CP} = 2.7)

Corrected assignments for ¹³C NMR data for **1e**
120.66 (d, 1C, C₄Ar–H, ⁴J_{CP} = 1.6)
139.43 (d, 1C, C₃Ar–H, ³J_{CP} = 2.7)

Incorrect assignment: “¹H NMR (500 MHz, 20 °C, CD₃CN): δ 1.31 (dd, 6H, CH(CH₃)(CH₃), ³J_{HH} = 7.0, ³J_{HP} = 15.2), 1.46 (dd, 6H, CH(CH₃)(CH₃), ³J_{HH} = 7.2, ³J_{HP} = 17.6), 2.45 (oct, 2H, CH(CH₃)₂, ³J_{HH} ≈ ²J_{HP} = 7.2), 6.69 (s, 1H, C₆Ar–H), 6.70 (ddd, 1H, C₃Ar–H, ³J_{HH} = 8.0, ⁴J_{HP} = 2.1, ⁵J_{HH} = 1.0), 7.12 (dd, 1H, C₄Ar–H, ³J_{HH} = 8.0, ⁵J_{HP} = 1.0). ¹³C{¹H} NMR (125.7 MHz, 20 °C, CD₃CN): δ 16.39 (d, 2C, CH(CH₃)(CH₃), ²J_{CP} = 1.9), 18.00 (d, 2C, CH(CH₃)(CH₃), ²J_{CP} = 2.7), 28.73 (d, 2C, CH(CH₃)(CH₃), ¹J_{CP} = 28.8), 110.44 (d, 1C, C₆Ar–H, ³J_{CP} = 13.5), 120.66 (d, 1C, C₃Ar–H, ³J_{CP} = 1.6), 131.74 (s, 1C, C₅Ar–Cl), 132.09 (d, 1C, C₂Ar–Ni, ²J_{CP} = 34.2), 139.43 (d, 1C, C₄Ar–H, ⁴J_{CP} = 2.7), 167.35 (d, 1C, C₁Ar–OP, ²J_{CP} = 12.8).”

Corrected assignment: “¹H NMR (500 MHz, 20 °C, CD₃CN): δ 1.31 (dd, 6H, CH(CH₃)(CH₃), ³J_{HH} = 7.0, ³J_{HP} = 15.2), 1.46 (dd, 6H, CH(CH₃)(CH₃), ³J_{HH} = 7.2, ³J_{HP} = 17.6), 2.45 (oct, 2H, CH(CH₃)₂, ³J_{HH} ≈ ²J_{HP} = 7.2), 6.69 (s, 1H, C₆Ar–H), 6.70 (ddd, 1H, C₄Ar–H, ³J_{HH} = 8.0, ⁴J_{HP} = 2.1, ⁵J_{HP} = 1.0), 7.12 (dd, 1H, C₃Ar–H, ³J_{HH} = 8.0, ⁴J_{HP} = 1.0). ¹³C{¹H} NMR (125.7 MHz, 20 °C, CD₃CN): δ 16.39 (d, 2C, CH(CH₃)(CH₃), ²J_{CP} = 1.9), 18.00 (d, 2C, CH(CH₃)(CH₃), ²J_{CP} = 2.7), 28.73 (d, 2C, CH(CH₃)(CH₃), ¹J_{CP} = 28.8), 110.44 (d, 1C, C₆Ar–H, ³J_{CP} = 13.5), 120.66 (d, 1C, C₄Ar–H, ⁴J_{CP} = 1.6), 131.74 (s, 1C, C₅Ar–Cl), 132.09 (d, 1C, C₂Ar–Ni, ²J_{CP} = 34.2), 139.43 (d, 1C, C₃Ar–H, ³J_{CP} = 2.7), 167.35 (d, 1C, C₁Ar–OP, ²J_{CP} = 12.8).”

2. In the ¹³C NMR data for compound **1k**, the C–P coupling patterns were incorrectly interpreted. This interpretation was discussed in the last part of the discussion and the data given in the Experimental section also needs to be corrected.

The last paragraph of the Results & discussion section (page 16166, left column, “Very informative coupling [...] detected at all”) should be disregarded.

The ¹³C NMR data for compound **1k**, given in the left column of page 16169, should be changed as follows:

Incorrectly assigned ¹³C NMR data for **1k**
125.16 (d, 1C, C₃Ar–H, ³J_{CP} = 12.1)
127.99 (d, 2C, *m*-C_{Ar}–H (Ph), ³J_{CP} = 139.5)
129.12 (d, 2C, *o*-C_{Ar}–H (Ph), ³J_{CP} = 106.8)
138.64 (d, 1C, C₅Ar–H, ³J_{CP} = 2.7)
139.78 (s, 1C, *p*-C_{Ar}–H (Ph))
C_qAr–Ar were not detected

Corrected assignments for ¹³C NMR data for **1k**
125.16 (d, 1C, C₆Ar–Ph, ⁴J_{CP} = 12.1)
127.43 (s, 1C, *p*-C_{Ar}–H (Ph)), 128.55 (s, 1C, C₅Ar–H)
128.69 (s, 2C, *m*-C_{Ar}–H (Ph)), 129.55 (s, 2C, *o*-C_{Ar}–H (Ph))
138.64 (d, 1C, C₃Ar–H, ³J_{CP} = 2.7)
139.78 (s, 1C, *ipso*-C_{Ar} (Ph))

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Incorrect assignment: $^{13}\text{C}\{^1\text{H}\}$ NMR (125.7 MHz, 20 °C, CD_3CN): δ 16.98 (d, 2C, $\text{CH}(\text{CH}_3)(\text{CH}_3)$, $^2J_{\text{CP}} = 1.9$), 18.50 (d, 2C, $\text{CH}(\text{CH}_3)(\text{CH}_3)$, $^2J_{\text{CP}} = 2.7$), 29.14 (d, 2C, $\text{CH}(\text{CH}_3)(\text{CH}_3)$, $^1J_{\text{CP}} = 29.4$), 122.21 (d, 1C, $\text{C}4_{\text{Ar}}\text{-H}$, $^4J_{\text{CP}} = 1.9$), 125.16 (d, 1C, $\text{C}3_{\text{Ar}}\text{-H}$, $^3J_{\text{CP}} = 12.1$), 127.99 (d, 2C, $m\text{-C}_{\text{Ar}}\text{-H}$ (Ph), $J_{\text{CP}} = 139.5$), 129.12 (d, 2C, $o\text{-C}_{\text{Ar}}\text{-H}$ (Ph), $J_{\text{CP}} = 106.8$), 135.65 (d, 1C, $\text{C}2_{\text{Ar}}\text{-Ni}$, $^2J_{\text{CP}} = 33.0$), 138.64 (d, 1C, $\text{C}5_{\text{Ar}}\text{-H}$, $^5J_{\text{CP}} = 2.7$), 139.78 (s, 1C, $p\text{-C}_{\text{Ar}}\text{-H}$ (Ph)), 163.78 (d, 1C, $\text{C}1_{\text{Ar}}\text{-OP}$, $^2J_{\text{CP}} = 12.6$), $\text{C}_{\text{qAr}}\text{-Ar}$ were not detected.”

Corrected assignment: $^{13}\text{C}\{^1\text{H}\}$ NMR (125.7 MHz, 20 °C, CD_3CN): δ 16.98 (d, 2C, $\text{CH}(\text{CH}_3)(\text{CH}_3)$, $^2J_{\text{CP}} = 1.9$), 18.50 (d, 2C, $\text{CH}(\text{CH}_3)(\text{CH}_3)$, $^2J_{\text{CP}} = 2.7$), 29.14 (d, 2C, $\text{CH}(\text{CH}_3)(\text{CH}_3)$, $^1J_{\text{CP}} = 29.4$), 122.21 (d, 1C, $\text{C}4_{\text{Ar}}\text{-H}$, $^4J_{\text{CP}} = 1.9$), 125.16 (d, 1C, $\text{C}6_{\text{Ar}}\text{-Ph}$, $^4J_{\text{CP}} = 12.1$), 127.43 (s, 1C, $p\text{-C}_{\text{Ar}}\text{-H}$ (Ph)), 128.55 (s, 1C, $\text{C}5_{\text{Ar}}\text{-H}$), 128.69 (s, 2C, $m\text{-C}_{\text{Ar}}\text{-H}$ (Ph)), 129.55 (s, 2C, $o\text{-C}_{\text{Ar}}\text{-H}$ (Ph)), 135.65 (d, 1C, $\text{C}2_{\text{Ar}}\text{-Ni}$, $^2J_{\text{CP}} = 33.0$), 138.64 (d, 1C, $\text{C}3_{\text{Ar}}\text{-H}$, $^3J_{\text{CP}} = 2.7$), 139.78 (s, 1C, $ipso\text{-C}_{\text{Ar}}$ (Ph)), 163.78 (d, 1C, $\text{C}1_{\text{Ar}}\text{-OP}$, $^2J_{\text{CP}} = 12.6$.”

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

