Dalton Transactions

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Dalton Trans.*, 2020, **49**, 6897

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

Loïc P. Mangin and Davit Zargarian *

DOI: 10.1039/d0dt90090g

rsc.li/dalton

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 $C3_{Ar}$–H and $C4_{Ar}$–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 ^{1}H NMR and ^{13}C data for compound **1e**, given in the left column of page 16168, should be changed as follows:

Incorrectly assigned ^{1}H NMR data for **1e**
6.70 (ddd, 1H, $C3_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{4}J_{HP}$ = 2.1, $^{5}J_{HH}$ = 1.0)
7.12 (dd, 1H, $C4_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{5}J_{HP}$ = 1.0)

Corrected assignments for ^{1}H NMR data for **1e**
6.70 (ddd, 1H, $C4_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{4}J_{HH}$ = 2.1, $^{5}J_{HP}$ = 1.0)
7.12 (dd, 1H, $C3_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{4}J_{HP}$ = 1.0)

Incorrectly assigned ^{13}C NMR data for **1e**
120.66 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 1.6)
139.43 (d, 1C, $C4_{Ar}$–H, $^{4}J_{CP}$ = 2.7)

Corrected assignments for ^{13}C NMR data for **1e**
120.66 (d, 1C, $C4_{Ar}$–H, $^{4}J_{CP}$ = 1.6)
139.43 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 2.7)

Incorrect assignment: "^{1}H NMR (500 MHz, 20 °C, CD_3CN): δ 1.31 (dd, 6H, CH(CH_3)(CH_3), $^{3}J_{HH}$ = 7.0, $^{3}J_{HP}$ = 15.2), 1.46 (dd, 6H, CH(CH_3)(CH_3), $^{3}J_{HH}$ = 7.2, $^{3}J_{HP}$ = 17.6), 2.45 (oct, 2H, C*H*(CH_3)$_2$, $^{3}J_{HH} \approx {}^{2}J_{HP}$ = 7.2), 6.69 (s, 1H, $C6_{Ar}$–*H*), 6.70 (ddd, 1H, $C3_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{4}J_{HP}$ = 2.1, $^{5}J_{HH}$ = 1.0), 7.12 (dd, 1H, $C4_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{5}J_{HP}$ = 1.0). ^{13}C{^{1}H} NMR (125.7 MHz, 20 °C, CD_3CN): δ 16.39 (d, 2C, CH(*C*H_3)(CH_3), $^{2}J_{CP}$ = 1.9), 18.00 (d, 2C, CH(CH_3)(*C*H_3), $^{2}J_{CP}$ = 2.7), 28.73 (d, 2C, *C*H(CH_3)(CH_3), $^{1}J_{CP}$ = 28.8), 110.44 (d, 1C, $C6_{Ar}$–H, $^{3}J_{CP}$ = 13.5), 120.66 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 1.6), 131.74 (s, 1C, $C5_{Ar}$–Cl), 132.09 (d, 1C, $C2_{Ar}$–Ni, $^{2}J_{CP}$ = 34.2), 139.43 (d, 1C, $C4_{Ar}$–H, $^{4}J_{CP}$ = 2.7), 167.35 (d, 1C, $C1_{Ar}$–OP, $^{2}J_{CP}$ = 12.8)."

Corrected assignment: "^{1}H NMR (500 MHz, 20 °C, CD_3CN): δ 1.31 (dd, 6H, CH(CH_3)(CH_3), $^{3}J_{HH}$ = 7.0, $^{3}J_{HP}$ = 15.2), 1.46 (dd, 6H, CH(CH_3)(*C*H_3), $^{3}J_{HH}$ = 7.2, $^{3}J_{HP}$ = 17.6), 2.45 (oct, 2H, C*H*(CH_3)$_2$, $^{3}J_{HH} \approx {}^{2}J_{HP}$ = 7.2), 6.69 (s, 1H, $C6_{Ar}$–*H*), 6.70 (ddd, 1H, $C4_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{4}J_{HH}$ = 2.1, $^{5}J_{HP}$ = 1.0), 7.12 (dd, 1H, $C3_{Ar}$–*H*, $^{3}J_{HH}$ = 8.0, $^{4}J_{HP}$ = 1.0). ^{13}C{^{1}H} NMR (125.7 MHz, 20 °C, CD_3CN): δ 16.39 (d, 2C, CH(*C*H_3)(CH_3), $^{2}J_{CP}$ = 1.9), 18.00 (d, 2C, CH(CH_3)(*C*H_3), $^{2}J_{CP}$ = 2.7), 28.73 (d, 2C, *C*H(CH_3)(CH_3), $^{1}J_{CP}$ = 28.8), 110.44 (d, 1C, $C6_{Ar}$–H, $^{3}J_{CP}$ = 13.5), 120.66 (d, 1C, $C4_{Ar}$–H, $^{4}J_{CP}$ = 1.6), 131.74 (s, 1C, $C5_{Ar}$–Cl), 132.09 (d, 1C, $C2_{Ar}$–Ni, $^{2}J_{CP}$ = 34.2), 139.43 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 2.7), 167.35 (d, 1C, $C1_{Ar}$–OP, $^{2}J_{CP}$ = 12.8)."

2. In the ^{13}C 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 ^{13}C NMR data for compound **1k**, given in the left column of page 16169, should be changed as follows:

Incorrectly assigned ^{13}C NMR data for **1k**
125.16 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 12.1)
127.99 (d, 2C, *m*-C_{Ar}–H (Ph), J_{CP} = 139.5)
129.12 (d, 2C, *o*-C_{Ar}–H (Ph), J_{CP} = 106.8)
138.64 (d, 1C, $C5_{Ar}$–H, $^{5}J_{CP}$ = 2.7)
139.78 (s, 1C, *p*-C_{Ar}–H (Ph))
C_{qAr}–Ar were not detected

Corrected assignments for ^{13}C NMR data for **1k**
125.16 (d, 1C, $C6_{Ar}$–Ph, $^{4}J_{CP}$ = 12.1)
127.43 (s, 1C, *p*-C_{Ar}–H (Ph)), 128.55 (s, 1C, $C5_{Ar}$–H)
128.69 (s, 2C, *m*-C_{Ar}–H (Ph)), 129.55 (s, 2C, *o*-C_{Ar}–H (Ph))
138.64 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 2.7)
139.78 (s, 1C, *ipso*-C_{Ar} (Ph))
—

Département de chimie, Université de Montréal, Montréal, Québec, Canada H3C 3J7. E-mail: zargarian.davit@umontreal.ca

Incorrect assignment: "$^{13}C\{^{1}H\}$ NMR (125.7 MHz, 20 °C, CD_3CN): δ 16.98 (d, 2C, $CH(CH_3)(CH_3)$, $^{2}J_{CP}$ = 1.9), 18.50 (d, 2C, $CH(CH_3)(CH_3)$, $^{2}J_{CP}$ = 2.7), 29.14 (d, 2C, $CH(CH_3)(CH_3)$, $^{1}J_{CP}$ = 29.4), 122.21 (d, 1C, $C4_{Ar}$–H, $^{4}J_{CP}$ = 1.9), 125.16 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 12.1), 127.99 (d, 2C, *m*-C_{Ar}–H (Ph), J_{CP} = 139.5), 129.12 (d, 2C, *o*-C_{Ar}–H (Ph), J_{CP} = 106.8), 135.65 (d, 1C, $C2_{Ar}$–Ni, $^{2}J_{CP}$ = 33.0), 138.64 (d, 1C, $C5_{Ar}$–H, $^{5}J_{CP}$ = 2.7), 139.78 (s, 1C, *p*-C_{Ar}–H (Ph)), 163.78 (d, 1C, $C1_{Ar}$–OP, $^{2}J_{CP}$ = 12.6), C_{qAr}–Ar were not detected."

Corrected assignment: "$^{13}C\{^{1}H\}$ NMR (125.7 MHz, 20 °C, CD_3CN): δ 16.98 (d, 2C, $CH(CH_3)(CH_3)$, $^{2}J_{CP}$ = 1.9), 18.50 (d, 2C, $CH(CH_3)(CH_3)$, $^{2}J_{CP}$ = 2.7), 29.14 (d, 2C, $CH(CH_3)(CH_3)$, $^{1}J_{CP}$ = 29.4), 122.21 (d, 1C, $C4_{Ar}$–H, $^{4}J_{CP}$ = 1.9), 125.16 (d, 1C, $C6_{Ar}$–Ph, $^{4}J_{CP}$ = 12.1), 127.43 (s, 1C, *p*-C_{Ar}–H (Ph)), 128.55 (s, 1C, $C5_{Ar}$–H), 128.69 (s, 2C, *m*-C_{Ar}–H (Ph)), 129.55 (s, 2C, *o*-C_{Ar}–H (Ph)), 135.65 (d, 1C, $C2_{Ar}$–Ni, $^{2}J_{CP}$ = 33.0), 138.64 (d, 1C, $C3_{Ar}$–H, $^{3}J_{CP}$ = 2.7), 139.78 (s, 1C, *ipso*-C_{Ar} (Ph)), 163.78 (d, 1C, $C1_{Ar}$–OP, $^{2}J_{CP}$ = 12.6)."

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