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McEllin, Alice Jane, Goult, Christopher A., Whitwood, Adrian C. et al. (2024) Erratum: Correction: On the mercuration, palladation, transmetalation and direct auration of a C^NC pincer ligand (Dalton transactions (Cambridge, England : 2003) (2023) 52 4 (872-876)). Dalton transactions (Cambridge, England : 2003). pp. 7641-7642. ISSN: 1477-9234

<https://doi.org/10.1039/d4dt90063d>

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Cite this: *Dalton Trans.*, 2024, **53**, 7641DOI: 10.1039/d4dt90063d
rsc.li/dalton

Correction: On the mercuration, palladation, transmetalation and direct auration of a C^NAC pincer ligand

Alice Jane McEllin,  Christopher A. Gault,  Adrian C. Whitwood, 
Jason M. Lynam  and Duncan W. Bruce *Correction for 'On the mercuration, palladation, transmetalation and direct auration of a C^NAC pincer ligand' by Alice Jane McEllin *et al.*, *Dalton Trans.*, 2023, **52**, 872–876, <https://doi.org/10.1039/d2dt04114f>.

In the original paper, **Fig. 3(b)** illustrates part of the ¹H NMR spectrum of 2,6-bis(2,2',3,3'-tetramethoxyppyridine) (3-1 in the original manuscript) relating to the resonances of the pyridyl hydrogens.

This resonance is complex when compared to the simple and expected AX₂ doublet and triplet seen in the related chlorogold(III) complexes (original manuscript **Fig. 3(c)**). We incorrectly attributed this complexity as originating in a diastereotopic relationship between the two *m*-hydrogens, which in turn we attributed as arising from the chiral nature of the *anti*-atropoisomer of the ligand. While this isomer of the ligand is indeed chiral (it possesses no improper axes of symmetry), we were mistaken in assigning the relationship between the *m*-hydrogen atoms which are in fact homotopic and not diastereotopic. As such, the complexity of the signal arises as evidently the ratio of the chemical shift difference ($\Delta\nu$) to the coupling constant (*J*) decreases in magnitude, resulting in resonances that appear as a second-order AB₂ spin system.¹

The original **Fig. 3(b)** spectrum (reproduced here as Fig. 1(a)) was recorded at 400 MHz and to support this revised (correct) interpretation, we re-recorded the ¹H NMR spectrum of 3-1 at 700 MHz, (shown here as Fig. 1(b)). While the spectrum recorded at higher field remains second order with considerable roofing, it is starting to approach the simple triplet and doublet signals that would be observed in the first-order spectrum, consistent with an increase in chemical shift difference at higher field.

In order to understand the origin of the effect, we undertook analysis of the spectrum of the ligand and its chlorogold(III) complex. Using the approach in ref. 1, we evaluated $\Delta\nu/J$ to be ≈ 2.6 for the ligand and ≈ 22.4 for the complex, explaining why the second-order effect is more pronounced in the ligand. Closer examination showed that the difference between the system arises due to changes in the chemical shift of the *m*-hydrogen atoms of the pyridine ring. They move from 8.31 ppm in the complex to 7.80 ppm in the ligand, with the chemical shift of the *p*-hydrogen remaining almost constant (7.84 ppm in the complex and 7.76 ppm in the ligand). The origin of this change in chemical shift would appear to arise as the steric effect of the methoxy groups in the 2,2'-positions ensure that the phenyl rings are twisted out of the plane of the pyridine ring (Fig. 2). The *m*-hydrogen atoms are then shielded by the phenyl ring current, leading to an upfield shift of *ca.* 0.5 ppm, which reduces $\Delta\nu/J$, causing the signal to become second order.

The error came to light during the refereeing of a subsequent manuscript² and we are grateful to one of the referees for bringing this issue to our attention.

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



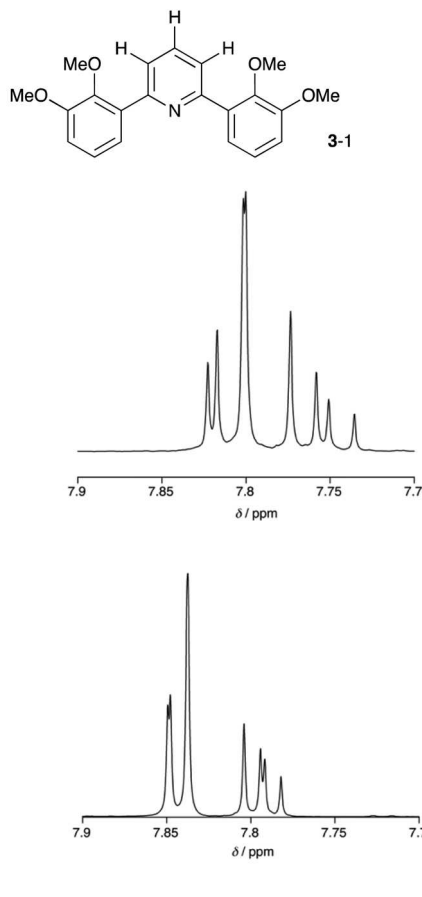


Fig. 1 ^1H NMR spectrum in the region of the pyridyl hydrogen atoms of compound 3-1 recorded at (a) 400 MHz and (b) 700 MHz.

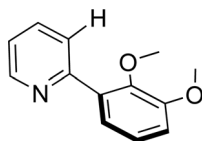


Fig. 2 Schematic diagram to show the *m*-hydrogen of the pyridine ring sitting over the phenyl ring, which is twisted out of plane.

References

- 1 J. W. Akitt and B. E. Mann, *NMR and Chemistry: An Introduction to Modern NMR Spectroscopy 4th Edn*, Stanley Thornes, Cheltenham, 2000, p. 76.
- 2 A. J. McEllin, C. A. Goult, G. Mohiuddin, L. J. Curtis, T. F. N. Tanner, A. C. Whitwood, J. M. Lynam and D. W. Bruce, *Inorg. Chem.*, 2024, DOI: [10.1021/acs.inorgchem.3c03791](https://doi.org/10.1021/acs.inorgchem.3c03791).

