## Chemical Science



## CORRECTION

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## Correction: HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes

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Correction for 'HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes' by Elisabetta Alberico *et al.*, *Chem. Sci.*, 2021, **12**, 13101–13119, DOI: 10.1039/D1SC04181A.

The authors regret that in Scheme 2 of the original article, complexes 7 and 8 were drawn incorrectly. The solid-state structure of both complexes, as established by X-ray analysis, had been previously reported (7 (ref. 1) and 8 (ref. 2)). In both complexes, the PNP ligand adopts a facial tridentate coordination to molybdenum and not a meridional one, as erroneously shown in Scheme 2 of the original article. The correct ligand arrangements in the metal coordination sphere for complexes 7 and 8 are reported below in Scheme 1.

Scheme 1 Mo-PNP complexes tested in the dehydrogenation of HCOOH.

Please note that complex 8 is also shown in Scheme 4 in the proposed mechanism for HCOOH decarbonylation (green part), and in Fig. 2. In both cases, the correct structure for complex 8 is reported below in Scheme 2 and Fig. 1.

NCCH<sub>3</sub> нсоон OC(O)H нсоон =OH HCOOнсоон - CO<sub>2</sub> - CO2 CH<sub>3</sub>OH + 5 (II) НСООН CO co 2 HCOOH 5-H<sub>2</sub> 3 HCO<sub>2</sub>H CH<sub>3</sub>OH H<sub>2</sub>O 2 CO2 OC(O)H 5-H<sub>2</sub>(II) DCOOD H<sub>2</sub>O -OCOH co 16-OCOH НСООН (II)

Scheme 2 Proposed mechanisms for HCOOH dehydrogenation (red), disproportionation (blue) and decarbonylation (green) promoted by 5. Evidence for the formation of a Mo(IV) species is based on the detection by NMR of  $H_2$  and HD following addition of DCOOD to  $Mo(H)_n$  species (see Fig. SI-31).

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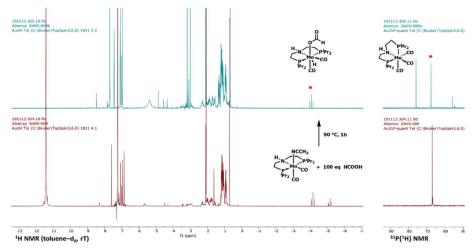


Fig. 1  $^{1}$ H and  $^{31}$ P( $^{1}$ H) NMR spectra of a toluene-d<sub>8</sub> solution of  $\{Mo(CH_{3}CN)(CO)_{2}(HN[(CH_{2}CH_{2}P)(CH(CH_{3})_{2})_{2}]_{2}\}$  4 in the presence of 100 equivalents of HCOOH ([Mo]  $10^{-2}$  M, [HCOOH] 1 M), before (a) and after heating at 90  $^{\circ}$ C for 1 hour (b). Spectra were recorded at room temperature. Signals related to complex 5 are marked by red dots.

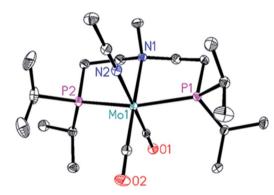


Fig. 2 Molecular structure of  $\{Mo(CO)_2(CH_3CN)[CH_3N(CH_2CH_2P(CH(CH_3)_2)_2)_2]\}$  9. Displacement ellipsoids correspond to 30% probability. Hydrogen atoms are omitted for clarity.

Furthermore, a mistake was made in the caption of Fig. 6, showing the solid-state structure of complex 9: the latter has been incorrectly described as a Mo(1)-hydride species  $\{Mo(H)(CO)_2(CH_3CN)[CH_3N(CH_2CH_2P(CH(CH_3)_2)_2)_2]\}$ . The correct formula, in agreement with the X-ray structure, is as follows and is shown above in Fig. 2:  $\{Mo(CO)_2(CH_3CN)[CH_3N(CH_2CH_2P(CH(CH_3)_2)_2)_2]\}$ . The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

## Notes and references

- 1 T. Leischner, A. Spannenberg, K. Junge and M. Beller, Synthesis of Molybdenum Pincer Complexes and Their Application in the Catalytic Hydrogenation of Nitriles, *ChemCatChem*, 2020, 12, 4543.
- 2 T. Leischner, A. Spannenberg, K. Junge and M. Beller, Molecular Defined Molybdenum–Pincer Complexes and Their Application in Catalytic Hydrogenations, *Organometallics*, 2018, 37, 4402.