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CORRECTION

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

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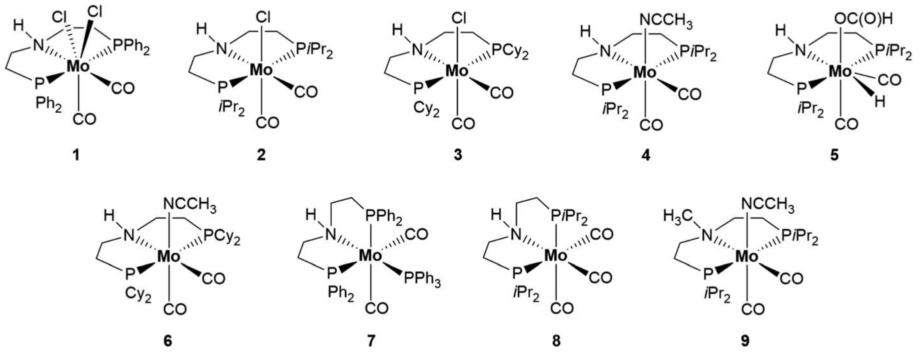
Correction for 'HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes' by Elisabetta Alberico *et al.*, *Chem. Sci.*, 2021, **12**, 13101–13119, DOI: 10.1039/D1SC04181A.

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.

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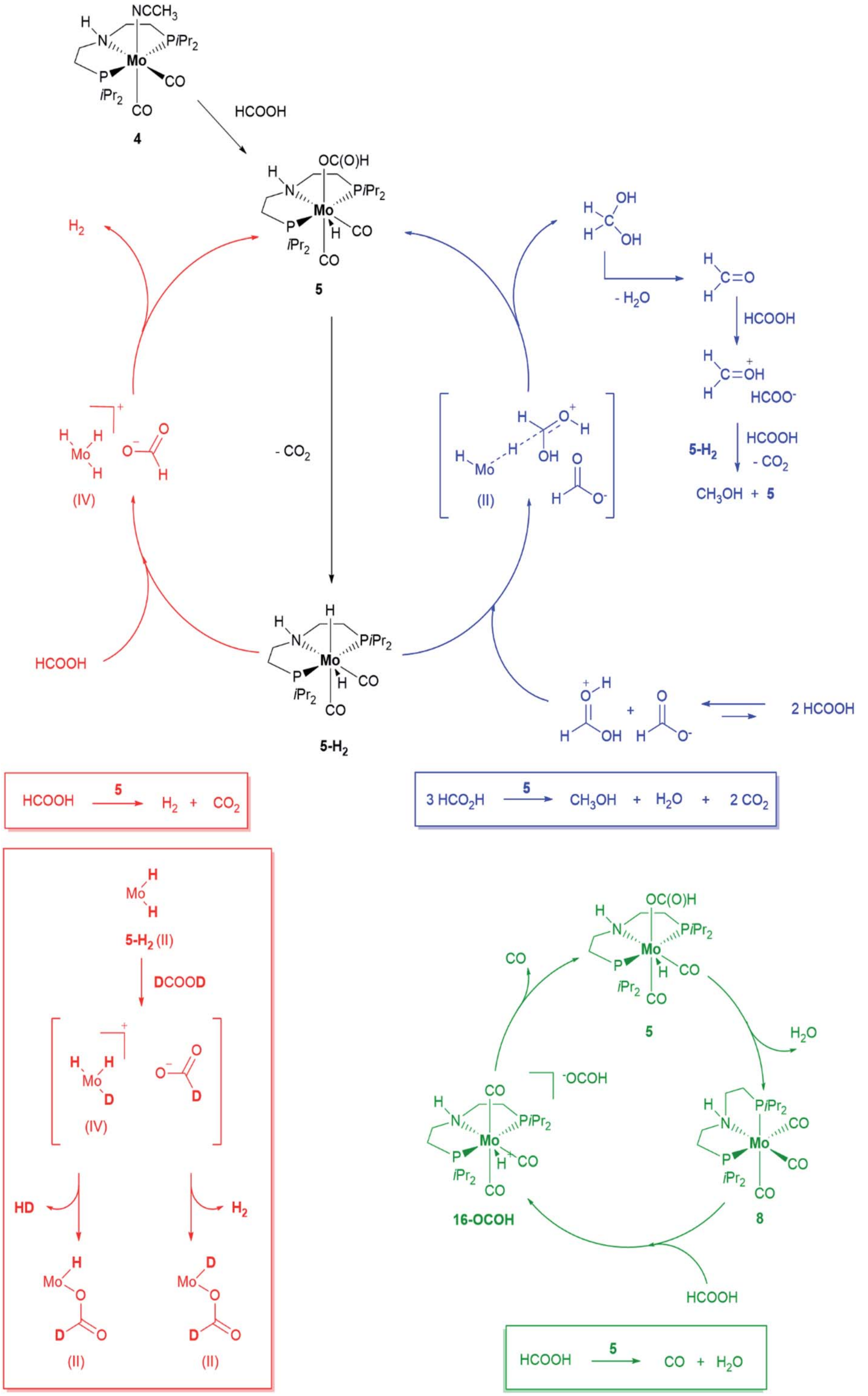
Please note that complex **8** is also shown in Scheme 4 in the proposed mechanism for HCOOH decarbonylation (green part), and in Fig. 2. In both cases, the correct structure for complex **8** is reported below in Scheme 2 and Fig. 1.



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).

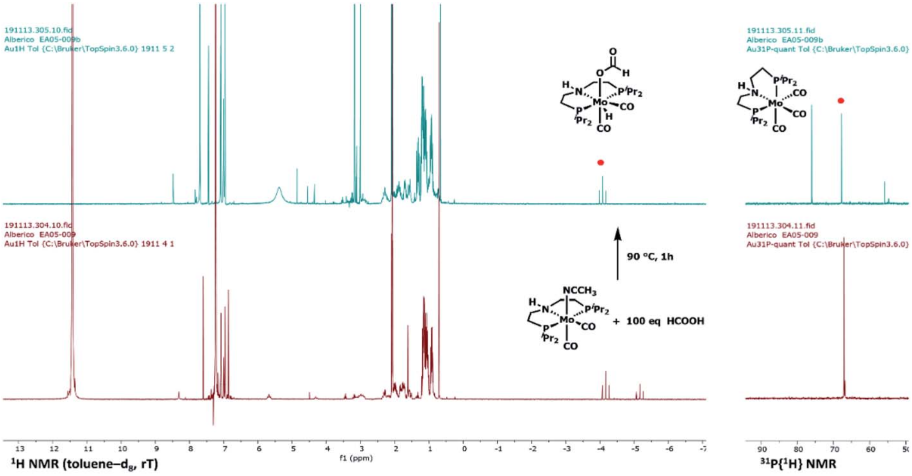


Fig. 1 $^1$H and $^{31}$P{$^1$H} NMR spectra of a toluene-d$_8$ solution of {Mo(CH$_3$CN)(CO)$_2$(HN[(CH$_2$CH$_2$P)(CH(CH$_3$)$_2$)$_2$]$_2$} **4** in the presence of 100 equivalents of HCOOH ([Mo] 10$^{-2}$ M, [HCOOH] 1 M), before (a) and after heating at 90 °C for 1 hour (b). Spectra were recorded at room temperature. Signals related to complex **5** are marked by red dots.

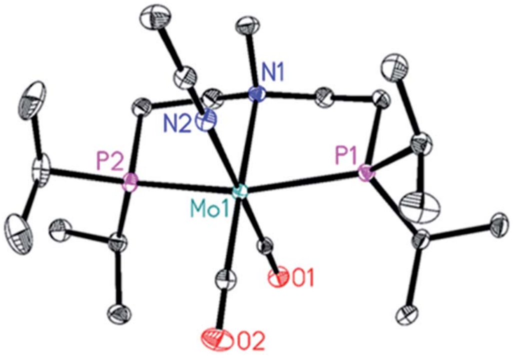


Fig. 2 Molecular structure of {Mo(CO)$_2$(CH$_3$CN)[CH$_3$N(CH$_2$CH$_2$P(CH(CH$_3$)$_2$)$_2$)$_2$]} **9**. Displacement ellipsoids correspond to 30% probability. Hydrogen atoms are omitted for clarity.

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(I)-hydride species {Mo(H)(CO)$_2$(CH$_3$CN)[CH$_3$N(CH$_2$CH$_2$P(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$_3$CN)[CH$_3$N(CH$_2$CH$_2$P(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.