

Correction: HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes

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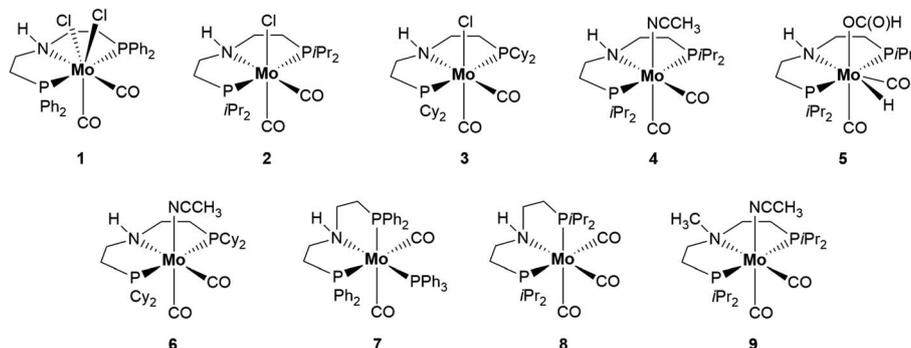
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Correction for 'HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes' by Elisabetta Alberico *et al.*, *Chem. Sci.*, 2021, 12, 13101–13119, DOI: 10.1039/D1SC04181A.

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.



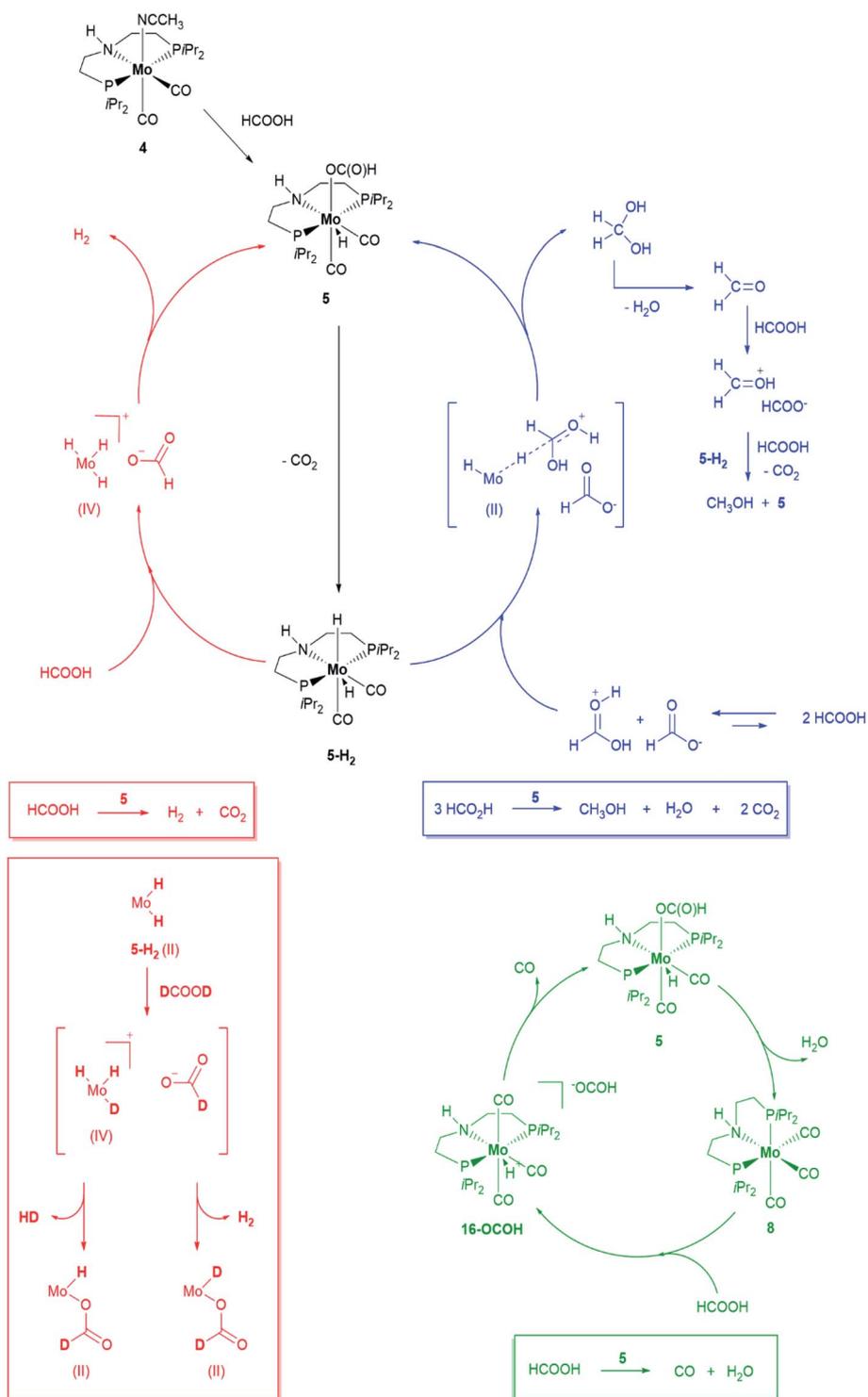
Scheme 1 Mo–PNP complexes tested in the dehydrogenation of HCOOH.

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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 H₂ and HD following addition of DCOOD to Mo(H)_n species (see Fig. SI-31).



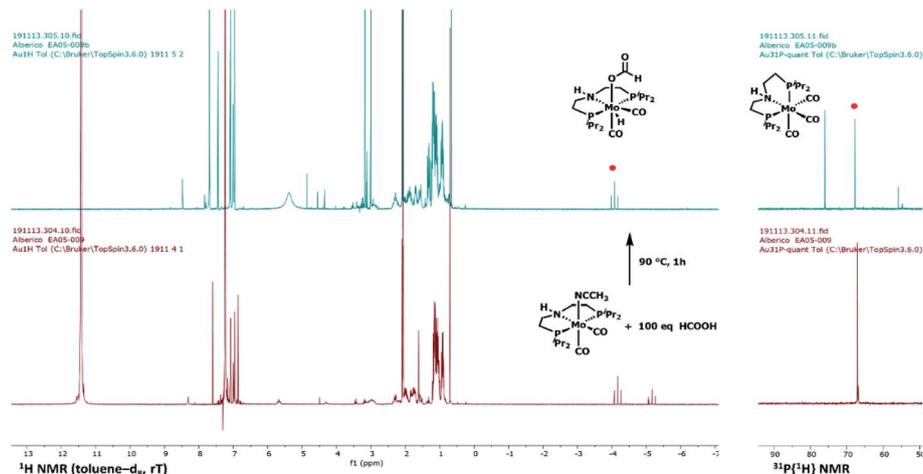


Fig. 1 ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of a toluene- d_8 solution of $\{\text{Mo}(\text{CH}_3\text{CN})(\text{CO})_2[\text{HN}[(\text{CH}_2\text{CH}_2\text{P})(\text{CH}(\text{CH}_3)_2)_2]_2\}$ **4** in the presence of 100 equivalents of HCOOH ($[\text{Mo}] 10^{-2} \text{ M}$, $[\text{HCOOH}] 1 \text{ M}$), 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.

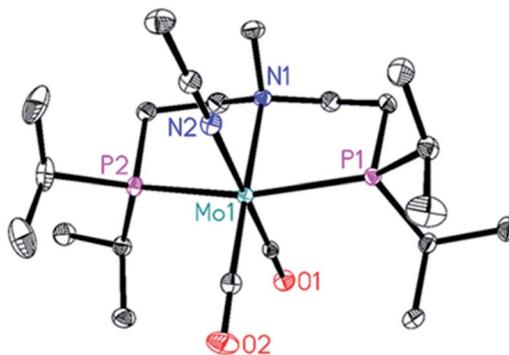


Fig. 2 Molecular structure of $\{\text{Mo}(\text{CO})_2(\text{CH}_3\text{CN})[\text{CH}_3\text{N}(\text{CH}_2\text{CH}_2\text{P}(\text{CH}(\text{CH}_3)_2)_2]_2\}$ **9**. Displacement ellipsoids correspond to 30% probability. Hydrogen atoms are omitted for clarity.

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 $\{\text{Mo}(\text{H})(\text{CO})_2(\text{CH}_3\text{CN})[\text{CH}_3\text{N}(\text{CH}_2\text{CH}_2\text{P}(\text{CH}(\text{CH}_3)_2)_2]_2\}$. The correct formula, in agreement with the X-ray structure, is as follows and is shown above in Fig. 2: $\{\text{Mo}(\text{CO})_2(\text{CH}_3\text{CN})[\text{CH}_3\text{N}(\text{CH}_2\text{CH}_2\text{P}(\text{CH}(\text{CH}_3)_2)_2]_2\}$.

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.

