

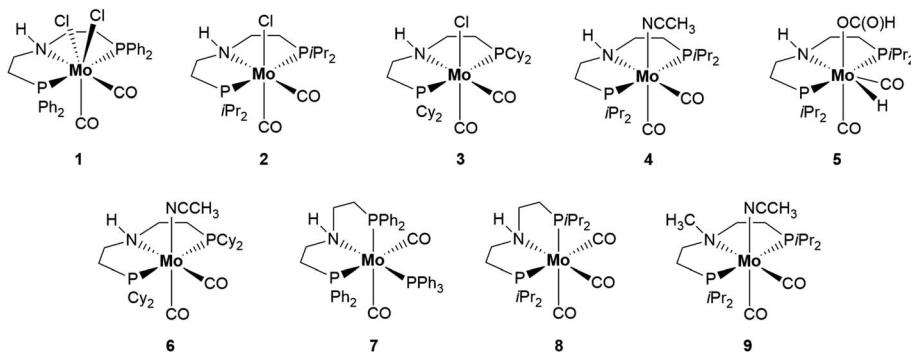
CORRECTION

View Article Online
View Journal | View IssueCite this: *Chem. Sci.*, 2021, **12**, 15772DOI: 10.1039/d1sc90239c
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Correction: HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes

Elisabetta Alberico,¹ Thomas Leischner,² Henrik Junge,¹ Anja Kammer,² Rui Sang,¹ Jenny Seifert,² Wolfgang Baumann,¹ Anke Spannenberg,² Kathrin Junge¹ and Matthias Beller¹Correction 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.

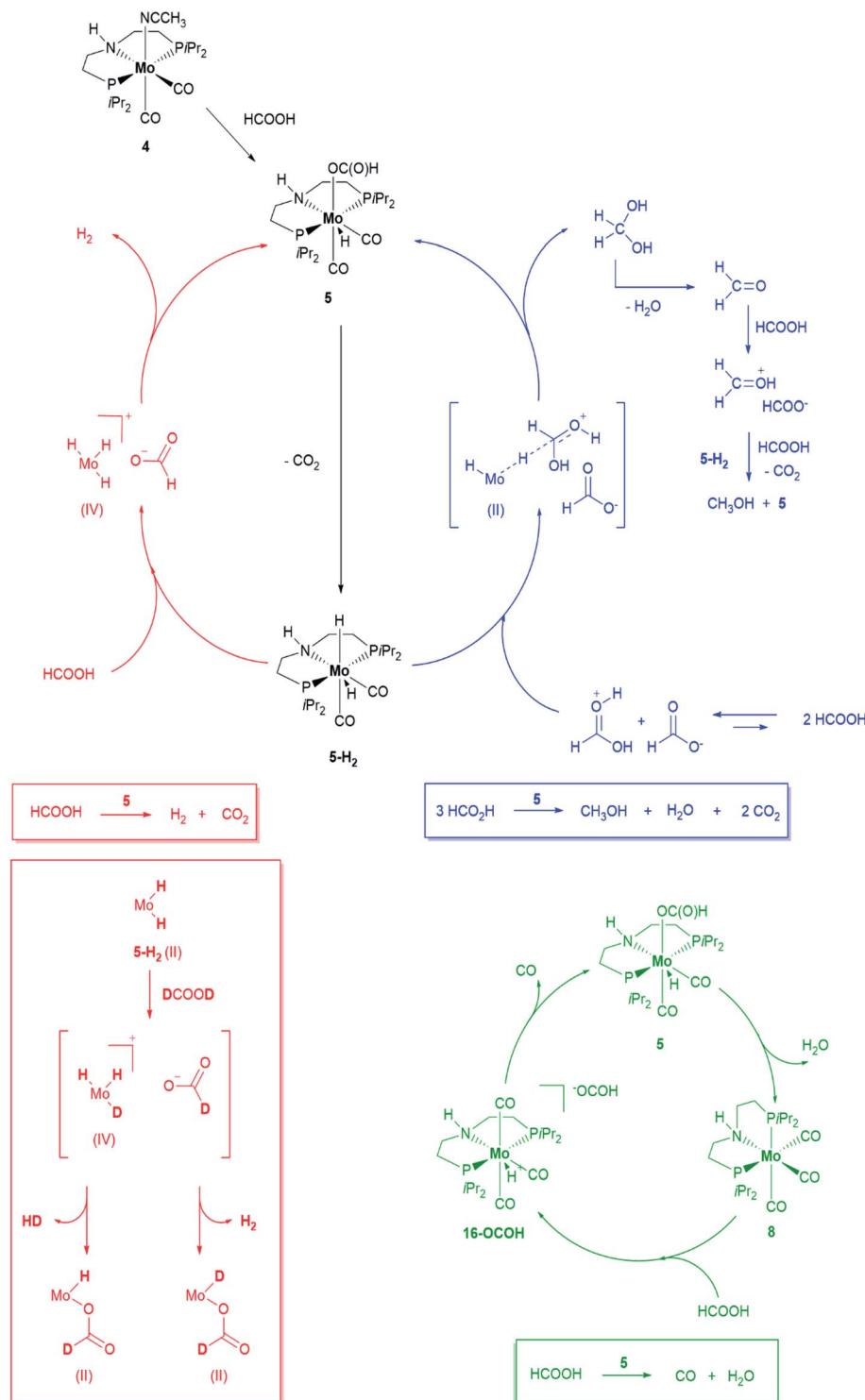
The authors regret that in Scheme 2 of the original article, complexes **7** and **8** were drawn incorrectly. The solid-state structure of both complexes, as established by X-ray analysis, had been previously reported (**7** (ref. 1) and **8** (ref. 2)). In both complexes, the PNP ligand adopts a facial 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 $\text{Mo}(\text{H})_n$ species (see Fig. SI-31).

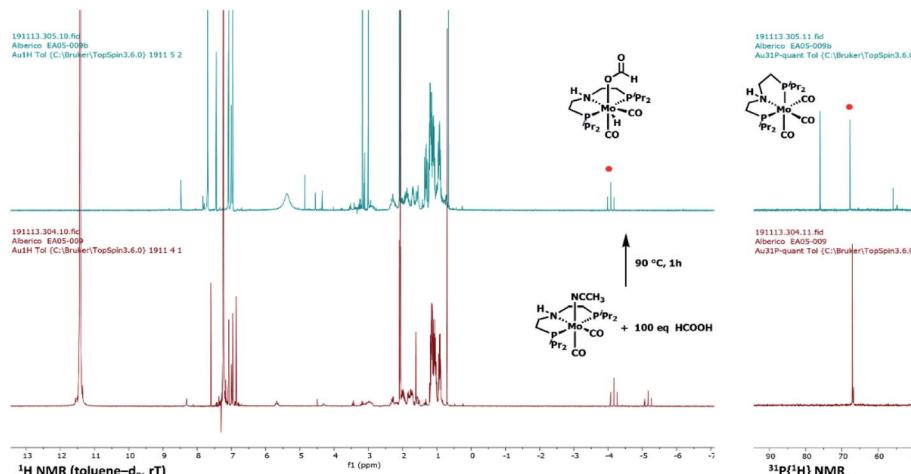


Fig. 1 ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of a toluene- d_8 solution of $\{\text{Mo}(\text{CH}_3\text{CN})(\text{CO})_2(\text{HN}[(\text{CH}_2\text{CH}_2\text{P})(\text{CH}(\text{CH}_3)_2)_2]_2\}$ 4 in the presence of 100 equivalents of HCOOH ($[\text{Mo}] = 10^{-2}$ M, $[\text{HCOOH}] = 1$ M), before (a) and after heating at $90\text{ }^\circ\text{C}$ for 1 hour (b). Spectra were recorded at room temperature. Signals related to complex 5 are marked by red dots.

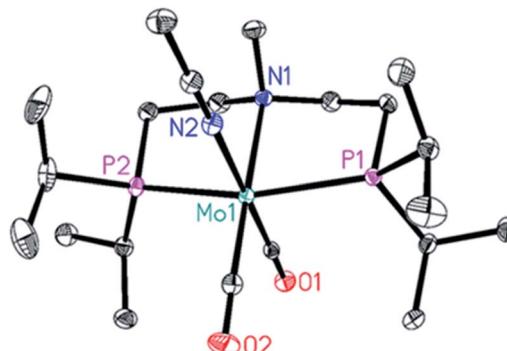


Fig. 2 Molecular structure of $\{\text{Mo}(\text{CO})_2(\text{CH}_3\text{CN})[\text{CH}_3\text{N}(\text{CH}_2\text{CH}_2\text{P}(\text{CH}(\text{CH}_3)_2)_2]_2\}$ 9. Displacement ellipsoids correspond to 30% probability. Hydrogen atoms are omitted for clarity.

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 $\{\text{Mo}(\text{H})(\text{CO})_2(\text{CH}_3\text{CN})[\text{CH}_3\text{N}(\text{CH}_2\text{CH}_2\text{P}(\text{CH}(\text{CH}_3)_2)_2]\}$. 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.

