

Correction to “Thermodynamic Analysis of Metal–Ligand Cooperativity of PNP Ru Complexes: Implications for CO₂ Hydrogenation to Methanol and Catalyst Inhibition”

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Supporting Information

Equation 13 in the Supporting Information contained a sign error, resulting in the incorrect pK_a values reported for (PNP)Ru–CO₂ and PNP. The pK_a of (PNP)Ru–CO₂ should be 26.1 ± 0.4 (not 24.6 ± 0.4). The pK_a of PNP should be 29.0 ± 0.4 (not 28.6 ± 0.4).

The same incorrect pK_a values are reported on page 14322, in the left column, last paragraph for PNP, and in the right column, first paragraph for (PNP)Ru–CO₂, and on page 14323, in Table 2, as well as in the SI (Table S3 and Figure S12 caption).

Also in the Supporting Information, Figures S15 and S17 have the wrong functions plotted. The slope of the correct function was used in extrapolating thermochemical parameters derived from Figure S17. The slope of Figure S15 was used to extrapolate thermochemical parameters, which resulted in our reporting incorrect values. The value of $K_{8,Cl}$ should be 0.004 ± 0.0016 (not 2.5×10^{-7}). The value of $K_{5,Cl}$ should be $2.0(\pm 0.8) \times 10^{-31}$ (not 1.3×10^{-34}), and hence the corresponding pK_a should be $>29.7 \pm 0.2$ (not $>33.9 \pm 0.4$). The value of $K_{6,Cl}$ should be $1.0(\pm 0.6) \times 10^{-7}$ (not 6.3×10^{-12}), and hence the corresponding $\Delta G_{6,Cl}$ should be 9.5 ± 0.3 kcal·mol^{−1} (not 15.3 ± 0.5 kcal·mol^{−1}).

A corrected Supporting Information file is provided that has revised versions of eq 13, Figure S12 caption, Figure S15, Figure S17, and Table S3. The corrected Table 2 is shown below.

Table 2. Summary of pK_a 's and Thermodynamic Parameters Pertinent to X[−] Release from (PNP)Ru–X

species	$pK_a^{a\ddagger}$	$K_{6,X}$ (M) ^{a†}	$\Delta G_{6,X}^0$ (kcal·mol ^{−1})
(PNP)	29.0 ± 0.4		
(PNP)Ru ⁺	20.7 ± 0.2		
(PNP)Ru–CO ₂	26.1 ± 0.4		
(PNP)Ru–OCHO	>25	2×10^{-3}	3.7 ± 0.7
(PNP)Ru–DMC	>32	9.6×10^{-11}	13.7 ± 0.7
(PNP)Ru–Cl	>29.7	1.0×10^{-7}	9.5 ± 0.3
(PNP)Ru–H		5.0×10^{-32}	42.7 ± 0.6

^{a†}Measurements were made at 20 °C. We assume that the equilibrium at 25 °C is approximately that at 20 °C.

None of these errors impact the discussion and conclusions drawn. We regret these errors and apologize for any confusion that may have resulted.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacs.1c06789>.

Experimental details, including syntheses, NMR and UV–vis data, and equilibrium plots (corrected) (PDF)

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