

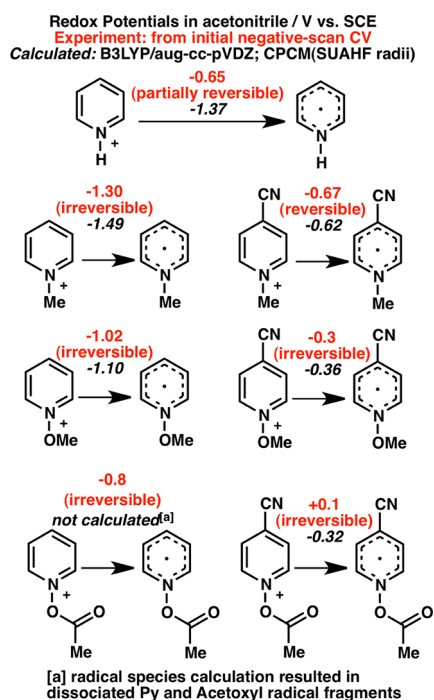
Correction to Theoretical Insights into Pyridinium-Based Photoelectrocatalytic Reduction of CO₂

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Page 7582. We correct the drawings of acetoxy-substituted pyridinium molecules and their calculated reduction potentials shown in Figure 2b of our original paper. After recognizing this error, we furthermore found that these species are a poor class of molecule to report since acetoxy radical fragments may irreversibly dissociate upon adding an electron to 1-acetoxy pyridinium molecules. Thus, the calculated values for those species are less likely to represent the experimentally reduced species.

The revised figure reports additional 1-electron redox potentials for 1-methoxy pyridinium species using the previous methodology. These values are in generally excellent agreement with experimental data by Lee and Kochi.¹ We also now explicitly report whether the experimental cyclic voltammetry measurements by Lee and Kochi were reversible or irreversible.



This correction does not change any of the conclusions in our paper, specifically that solvated 1-H pyridinium is a significant outlier compared to other calculated 1-electron reduction potentials, indicating that the measured reduction potential does not reflect homogeneous reduction of pyridinium but rather reduction of an adsorbed species.

REFERENCES

(1) Lee, K. Y.; Kochi, J. K. *J. Chem. Soc., Perkin Trans. 2* **1992**, 1011–1017.

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