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Mechanism of Photochemical N2 Reduction

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Data Management Plan

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Data types and sources

The data produced is concerned with the characterization of enzymes, their metal centers, spectroscopy, and kinetics of catalysis. The data is primarily numerical and includes gas chromatography, visible absorption, infrared, EPR and ENDOR spectra, mass spectra, cyclic voltammograms, and kinetic data. Collaborative studies provide computational results, elemental analyses, additional mass spectra, and additional EPR and ENDOR spectra.

Content and format

A narrative of data collection in the PI's lab is recorded in hardcopy notebooks, including the salient data results. Instrument-generated data, such as spectra, are stored in hard copies as printouts and/or instrument outputs, in addition to electronic versions such as ASCII codes, CSV files, MS Office documents, or other data-appropriate formats. All data is indexed in the hardcopy notebooks as a part of the research narrative.

Sharing and preservation

Access to obtained/produced data is made available to the public through scientific publications and poster and oral presentations. Where appropriate, tabulated data (DFT calculations), crystallographic (.cif) and picture (such as .tif and .jpeg) format files are presented in the supplementary information for published material. Data is not posted on a website or made available to the public via a database prior to publication. It is not anticipated that data will be deposited in databases that mine the published literature (e.g. PubChem, NIST Chemistry WebBook). In general the PI's lab will make available unpublished data to an interested party if that data is not being held confidential for intellectual property reasons.

Protection

The PI does not post data (published or unpublished) on a website or any other available venues for general access. Links to published work are made available on the website, with no disclaimers or terms of use, as these are determined by the journal where the data is published.

Rationale

All data generated in the PI's lab is stored for at least three years beyond the end of any funding period. To protect against water and fire damage, hardcopy notebooks, printouts of spectra or instrument outputs, and CD/DVD archives are stored on elevated metal shelving in a room with fire-stop doors separating it from any research laboratory. Electronic data storage devices include instruments' internal memory, external hard drives, and CD/DVD discs. As a regular practice, stored data is/will be periodically transferred to a new storage media to ensure compatibility with

emerging technologies. Additionally, a periodic full back-up of all electronic data is conducted and stored on an external hard-drive in a separate building, or on an external server (e.g., Box). Physical samples are stored in fireproof cabinets. Air-sensitive samples are kept in an inert atmosphere glovebox. Frozen samples are stored in liquid nitrogen dewars and -80C freezers, all fitted with alarms.