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New Strategies for Investigating Oxidative Aliphatic Carbon-carbon Bond Cleavage Reactions

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The data produced in the PI's laboratory is concerned with the characterization of compounds and analyzing their reactivity in a variety of chemical systems. The data is primarily numerical and includes NMR spectra (^{1}H and heteronuclear; one and two-dimensional), infrared and UV-vis spectra, EPR spectra, mass spectra, gas chromatograms, cyclic voltammograms, and UV-vis kinetic data Collaborative studies provide X-ray diffraction patterns, computational results, elemental analyses, additional mass spectra, and additional EPR spectra.

2.   **Data 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 such as .cif files for X-ray crystallography. All data is indexed in the hardcopy notebooks as a part of the research narrative.

3.   **Access to Data and Data Sharing Practices and Policies**

Access to obtained/produced data is made available to the public through scientific publications and poster and oral presentations. Additionally, all X-ray crystallographic structures accepted for publications are deposited in Cambridge Crystallographic Data Centre. 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 In general the PI's lab will make available unpublished data to an interested party if that data is not being held confidential for intellectual property reasons.

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5.   **Archiving of Data**

All data generated in the PI's lab is stored for at least three years beyond the end of any NSF 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. Physical samples are stored in fireproof cabinets. Air-sensitive samples are kept in an inert atmosphere glovebox.