

SAMUEL PETER SMITH

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Education

Doctor of Philosophy in Chemistry

The University of New Mexico

Expected December **2027**

Albuquerque, NM

- Committee Chair and Research Advisor: Jeffrey R. Rack, Ph.D.

Bachelor of Arts in Chemistry

The University of New Mexico

2022

Albuquerque, NM

Research Experience

Graduate Chemistry Research Assistant

The University of New Mexico

2022–2027

Albuquerque, NM

Advisor: Jeffrey R. Rack

- Redeveloped lab-built circular dichroism (CD) / magnetic circular dichroism (MCD) instrumentation to extend measurements into the near-UV. Reconfigured the optical layout and polarization optics to optimize fluence and suppress polarization artifacts enabling reliable differential absorption measurements of weak optical signals.
- Reimplemented transient absorption spectroscopy acquisition and analysis workflows in python for pump-probe measurements with variable pump wavelengths and dispersive probe detection. Developed software control for coordinated operation of discrete hardware components, including delay-stage positioning, optical chopper timing, spectrometer readout, pump/probe sequencing, shot-to-shot normalization, and automated data storage. Improved acquisition toward near shot-noise-limited detection and redesigned pulse-sequence handling to support future compatibility with pulse-to-pulse polarization modulation.
- Separated and characterized enantiomeric chiral sulfoxides as model systems for photochemical inversion at a trigonal-pyramidal chiral center. Used chiral HPLC to resolve enantiomers and steady-state CD spectroscopy to confirm enantiomeric resolution. Performed femtosecond transient absorption measurements that revealed short- and long-lived excited-state features tentatively assigned to singlet and triplet manifolds.
- Investigated magneto-optical activity in porphyrin complexes with systematically varied peripheral substituents, metal centers, and molecular symmetry. Collected and analyzed absorption and MCD spectra to determine how fluorination, electronic structure, and metal substitution tune MCD intensity and sign. Results form the basis of a manuscript in preparation for submission.
- Performed DFT and TDDFT calculations to support interpretation of optical and magneto-optical spectra in metal complexes and porphyrins. Used ORCA and Gaussian to assign electronic transitions, compare calculated spectra with experimental absorption and MCD spectra, and evaluated vibronic contributions to spectra using excited-state dynamics modules. Calculations contributed to a peer-reviewed publication in *Inorganic Chemistry*.
- Developed Python workflows for spectral processing, kinetic analysis, fitting, and publication-quality visualization using packages such as NumPy, pandas, SciPy, matplotlib, and lmfit. Built reusable tools for fitting and plotting absorption, CD, MCD, and transient absorption datasets. These workflows became standard tools within the research group and are maintained as open-source packages.
- Mentored undergraduate researchers in molecular spectroscopy, sample preparation, Python-based data analysis, and safe laboratory practices.

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Teaching & Mentoring Experience

Graduate Teaching Assistant – Undergraduate Inorganic Chemistry

2023

The University of New Mexico, Department of Chemistry and Chemical Biology

Albuquerque, NM

- Supported instruction for an upper-division inorganic chemistry course covering atomic structure, molecular symmetry and group theory, bonding models, coordination chemistry, spectroscopy, acid-base and redox chemistry, main-group trends, organometallic chemistry, catalysis, f-block chemistry, and materials chemistry.
- Led problem-solving support and office-hour instruction for topics including symmetry operations, character tables, vibrational spectroscopy, ligand-field theory, and coordination-complex electronic structure.
- Assisted with grading, student feedback, exam preparation, and conceptual review for a broad senior-level course integrating physical and inorganic chemistry.

Graduate Teaching Assistant – Advanced Synthetic Chemistry Laboratory

2024

The University of New Mexico, Department of Chemistry and Chemical Biology

Albuquerque, NM

- Supervised students in a capstone undergraduate laboratory focused on multi-step organic and inorganic synthesis, experimental design, and modern chemical characterization.
- Trained students in safe laboratory technique, professional notebook-keeping, and interpretation of FT-IR, UV-vis, NMR, GC-MS, cyclic voltammetry, and mass spectrometry data.
- Guided students in writing comprehensive laboratory reports in the style of professional publications and presenting chemical results to a broad audience.
- Supported development of independent laboratory skills, including literature research, troubleshooting synthetic procedures, assessing product purity, and connecting spectroscopic data to molecular structure.

Graduate Teaching Assistant – Mass Spectrometry Facility

2025–present

The University of New Mexico, Department of Chemistry and Chemical Biology

Albuquerque, NM

- Trained undergraduate and graduate users in sample preparation, LC-MS instrument operation, and interpretation of mass spectrometry data.
- Supported educational outreach by mentoring high school students involved in statewide science fair activities, introducing students to analytical chemistry, mass spectrometry concepts, and scientific data interpretation.

Publications

Electron withdrawing meso-substituents turn-on magneto-optical activity in Porphyrins. Emigdio Turner, Trong-Nhan Pham, Samuel Smith, Kaytlin Ward, Joel Rosenthal, Jeffrey Rack. *Inorganic Chemistry* (2024). 2024

Presentations

Smith, S.P. Brink, J. Rack, J.J. Changing Porphyrin Symmetry Reverses Magneto-Optical Rotation. Presented at the Rocky Mountain Regional Meeting of the American Chemical Society, Albuquerque, NM, Oct, 2025; Poster.

Smith, S.P. Quartey, E. Breen, D.J. Rack, J.J. When Does Inversion Occur in Chiral Sulfoxides? Conference on Excited State Processes. Santa Fe, NM, June 16, 2025; Poster.