Partial Charge Determination of SC-XRD Data with Refinement of Occupancy of Spherical Atoms (ROSA)

Taylor Keller[1], Alex Byrne[2], Michael Zdilla[3]

[1]Temple University [2]Temple University, [3]Chemistry, Temple Univ

tmkeller@temple.edu

Crystallography is at the forefront of emerging research in determining partial atomic charges. Currently exceptional datasets with high resolution and signal-to-noise are required for charge elucidation in addition to advanced techniques and software that include charge density refinement, non-spherical atomic form factors, and/ or combinations of quantum mechanical calculations. We introduce a simple and user-friendly experimental approach in determining partial atomic charges using single crystal diffraction data with Refinement of Occupancy of Spherical Atoms (ROSA). Included are comparisons of ROSA charges with more sophisticated methods pioneered by Coppens, encoded in MoPro, and high-level quantum calculations.