Radiolytic Damage in Small-Molecule 3D Electron Crystallography

Ambarneil Saha[1], Niko Vlahakis[2], Jose Rodriguez[3]

[1]University of California, Los Angeles [2]University of California, Los Angeles, [3]UCLA

asaha@chem.ucla.edu

Every electron diffraction experiment is fundamentally limited by radiation damage. Immediately as the crystal of interest is illuminated by the incident beam, a complex set of inelastic scattering events initiates a cascade of radiolytic reactions within the sample, breaking chemical bonds and ultimately destroying the structural integrity of the crystal lattice. In 3D electron crystallography, an irradiated specimen is unidirectionally rotated within a transmission electron microscope while reciprocal space is periodically sampled in regular intervals, generating a tomographic series of diffraction patterns. Here we analyze a series of diffraction datasets acquired from repeated, consecutive sampling of single nanocrystals formed by organic and organometallic compounds. These species represent groups of small-molecule structures featuring site-specific modifications to an otherwise conserved scaffold. Our results indicate that chemically inspired substitutions can exert a significant effect on either accelerating or arresting the onset and progression of radiolytic damage, thus diminishing or enhancing the dose tolerance of specific crystalline specimens. Motifs explored include loss of aromaticity and removal of heavier atoms with relatively favorable elastic-to-inelastic cross-section ratios.