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X-rays, Action, Camera! The Joys and Heartaches of Making Movies of Redox Enzymes in Motion. Carrie M. Wilmot, Dept. of Biochemistry, Molecular Biology & Biophysics, Univ. of Minnesota, Minneapolis, MN 55455.

Except in rare cases, X-ray crystal structures of enzymes are at the resolution of medium sized atoms, not the individual electrons/protons that reveal the details of catalysis. In contrast, various spectroscopic techniques are very good at defining the positions of electrons/protons. By combining crystallography and spectroscopy a level of structural insight can be achieved that has never before been possible. Many enzymes are catalytically active in the crystal, and due to the restraints imposed by the crystal lattice the rates of individual reaction steps are often slower than in solution. This means that transient reaction intermediates that have been difficult to characterize in solution, build up to accessible levels in crystals. By running kinetics in crystals, the extraordinary potential to “see” these intermediates, and then solve their structures to near atomic resolution, is enormous. Flash freezing is used to press the “pause” button on the enzymatic reaction in the crystal, while spectroscopy ensures the correct assignment of the catalytic state of the crystalline enzyme, and allows the resulting X-ray crystal structure “snapshot” to be precisely placed along the reaction co-ordinate to build up a “movie” of catalysis at the molecular level.