KN-3 High pressure synchrotron radiation crystallography, from organic conductors to chemistry in the lower mantle

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ID09A is a state of the art high pressure diffraction beamline at the ESRF. It uses monochromatic diffraction with large area detectors. Powder and single crystal diffraction experiments can be performed at high pressures in diamond anvil cells, permitting accurate determination of crystallographic properties of the investigated samples. Soon ID09A will be replaced by a new and improved beamline, ID15B. Recent technical advances have significantly added to the utility of single crystal X-ray diffraction experiments at high pressures [1]. New ways of supporting diamond anvils, like Boehler Almax anvils [2], have considerably increased the volume of accessible reciprocal space. Use of Helium or Neon as pressure transmitting medium extends substantially the practicable pressure range. Flat panel detectors have noticeably decreased the data collection time and increased the accuracy. Data can be collected at low and high temperatures. Even single crystal diffraction experiments with laser heating have become possible [3]. Here we will present several examples to illustrate the recent progress.

Work performed in collaboration with M. Merlini, Universitá degli Studi di Milano, Italy

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KN-4 Structure and mechanism of respiratory complex I, a giant molecular proton pump

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NADH-ubiquinone oxidoreductase (complex I) is the first and largest enzyme in the respiratory chain of mitochondria and many bacteria. It couples electron transfer between NADH and ubiquinone to the translocation of four protons across the membrane. It is a major contributor to the proton flux used for ATP generation in mitochondria, being one of the key enzymes essential for life as we know it. Mutations in complex I lead to the most common human genetic disorders. It is an L-shaped assembly formed by membrane and hydrophilic arms. Mitochondrial complex I consists of 44 subunits of about 1 MDa in total, whilst the prokaryotic enzyme is simpler and generally consists of 14 conserved “core” subunits. We use the bacterial enzyme as a “minimal” model to understand the mechanism of complex I. We have determined the first atomic structures of complex I, starting with the hydrophilic domain, followed by the membrane domain and, finally, the recent structure of the entire Thermus thermophilus complex (536 kDa, 16 subunits, 9 Fe-S clusters, 64 TM helices). Structures suggest an unusual mechanism of coupling between electron transfer in the hydrophilic domain (involving ~ 90 Å long chain of 7 conserved Fe-S clusters) and proton translocation in the membrane domain, via long-range (up to ~200 Å) conformational changes. It resembles a steam engine, with coupling elements (akin to coupling rods) linking parts of this molecular machine. I will discuss our current work, which is aimed at elucidating the molecular details of the coupling mechanism through determination of structures of the complex in different redox states with various bound substrates/inhibitors, using both X-ray crystallography and new cryo-EM methods.

Keywords: respiratory complex I, giant molecular proton pump