X-ray Induced Changes in Organic and Biological Crystalline Materials

Fabrice Camus[a], C. Besnard[a], M. Fleurant[a], I. Margiolaki[b], P. Pattison[a,c], M. Schiltz[a], [a]*Laboratory of Crystallography, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland.* [b]*ESRF, Grenoble, France.* [c]*Swiss-Norwegian Beamlines, ESRF, Grenoble, France.* E-mail: fabrice.camus@epfl.ch

The investigation of radiation-induced processes in organic and biological molecules is of importance for gaining a better understanding of the fundamental mechanisms by which certain compounds (*e.g.* halogenated nucleotides) induce a radio-sensitizing action and can thus be used to improve anticancer radiotherapies. The study of radiation-induced processes in macromolecules is also of considerable interest in the fields of structural biology and genomics, since current progress in synchrotron protein crystallography is hampered by radiation damage in the samples.

We have carried out powder diffraction measurements to investigate structural changes as a function of X-ray irradiation in organic and biological crystals. In these experiments, synchrotron radiation is used to both irradiate the samples and collect diffraction data. Powder diffraction is employed to monitor changes in the unit cell and microstructural parameters (crystallite size and lattice strain) in crystals of native and halogenated nucleobases as well as on other small-molecule model compounds under X-ray irradiation. Similar experiments were also carried out on macromolecular crystals. Our aim in these studies is to investigate radiation-induced changes as a function of temperature, wavelength and X-ray dose rate. Attempts to interpret the observed unit-cell expansions in terms of radiation-induced structural modifications in the crystal will be discussed.

Keywords: synchrotron powder diffraction, radiation chemistry, radiation damage studies