
Concluding Remarks

Time-resolved chemistry: from structure to function. A summary

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Never have I hitherto participated in a Faraday Discussion (over a period of nearly forty years) in which such an enormous range of techniques and such a wide variety of distinct phenomena were displayed. I therefore embark on this summary with some trepidation, as I do not feel adequate to the task required. Forgive me for giving a rather subjective account which inevitably reflects my own tastes, predilections and preferences—even though I have tried conscientiously to reflect a balanced view.

So far as techniques in general are concerned, it is obvious that faster and ever-more powerful lasers are key features of the time-resolved landscape, and will remain so for as long as one is interested in processes exhibiting shorter and shorter lifetimes. Synchrotron radiation is likewise well-nigh indispensable nowadays as a means of probing the course of both ultra-fast and also very slow processes. (I should like to insert parenthetically that about five or six years ago I heard a group of some of the UK's leading organic chemists declaring that chemistry, and its growth, could flourish perfectly well without synchrotrons. Only an intellectual Luddite would now hold that opinion, in view of the dramatic advances that have been reported at this meeting alone.)

Synchrotrons serve us best when we use them to record more than one kind of measurement—as I myself have found to my advantage ever since, with collaborators at Daresbury, we carried out parallel studies of our solid catalysts (*in situ*) using X-ray absorption spectroscopy and X-ray diffraction.¹ We heard from Evans *et al.* how much progress there has been recently (and of yet further expected advances) in employing dispersive EXAFS for investigating rapid reactions of transition-metal complexes in solution. Insofar as radically new departures are concerned, the dramatic, unconventional experiment proposed by Moffat involving so-called chirped X-ray pulses merits serious consideration. If one is to attain sub-picosecond (say 100 fs) resolution using synchrotron sources—and such time-scales are necessary to match or compete with what can be done by ultra-fast laser sources in tracking processes such as the rupture and formation of chemical bonds or some electron transfer processes—it follows inexorably that the Laue technique must be implemented. A supreme advantage in doing a time-resolved Laue diffraction experiment in this way (if it can be achieved) is that an energy-chirped pulse maps time into space. One hopes that the proposals made by Moffat can indeed be realised, as they will be of great value to the community of macromolecular crystallographers well represented at this Discussion.

When it comes to the study of excited states in solids, or probing the course of chemical changes in enzymes, Laue diffraction seems to offer major advantages which were also adumbrated by Moffat, and highlighted in the reflective Introductory Lecture by Coppens. (A recent comprehensive review² contains many key items of information concerning this approach). You will recall that, after the interesting presentation by Cole *et al.*, there was a lively debate as to whether future

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