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## 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.<sup>1</sup> 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 review<sup>2</sup> 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

# Time Resolved Chemistry From Structure To Function

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## **Table of Contents Time Resolved Chemistry From Structure To Function**

1. Understanding the eBook Time Resolved Chemistry From Structure To Function
  - The Rise of Digital Reading Time Resolved Chemistry From Structure To Function
  - Advantages of eBooks Over Traditional Books
2. Identifying Time Resolved Chemistry From Structure To Function
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Time Resolved Chemistry From Structure To Function
  - User-Friendly Interface
4. Exploring eBook Recommendations from Time Resolved Chemistry From Structure To Function
  - Personalized Recommendations
  - Time Resolved Chemistry From Structure To Function User Reviews and Ratings
  - Time Resolved Chemistry From Structure To Function and Bestseller Lists
5. Accessing Time Resolved Chemistry From Structure To Function Free and Paid eBooks

- Time Resolved Chemistry From Structure To Function Public Domain eBooks
  - Time Resolved Chemistry From Structure To Function eBook Subscription Services
  - Time Resolved Chemistry From Structure To Function Budget-Friendly Options
6. Navigating Time Resolved Chemistry From Structure To Function eBook Formats
    - ePub, PDF, MOBI, and More
    - Time Resolved Chemistry From Structure To Function Compatibility with Devices
    - Time Resolved Chemistry From Structure To Function Enhanced eBook Features
  7. Enhancing Your Reading Experience
    - Adjustable Fonts and Text Sizes of Time Resolved Chemistry From Structure To Function
    - Highlighting and Note-Taking Time Resolved Chemistry From Structure To Function
    - Interactive Elements Time Resolved Chemistry From Structure To Function
  8. Staying Engaged with Time Resolved Chemistry From Structure To Function
    - Joining Online Reading Communities
    - Participating in Virtual Book Clubs
    - Following Authors and Publishers Time Resolved Chemistry From Structure To Function
  9. Balancing eBooks and Physical Books Time Resolved Chemistry From Structure To Function
    - Benefits of a Digital Library
    - Creating a Diverse Reading Collection Time Resolved Chemistry From Structure To Function
  10. Overcoming Reading Challenges
    - Dealing with Digital Eye Strain
    - Minimizing Distractions
    - Managing Screen Time
  11. Cultivating a Reading Routine Time Resolved Chemistry From Structure To Function
    - Setting Reading Goals Time Resolved Chemistry From Structure To Function
    - Carving Out Dedicated Reading Time
  12. Sourcing Reliable Information of Time Resolved Chemistry From Structure To Function
    - Fact-Checking eBook Content of Time Resolved Chemistry From Structure To Function
    - Distinguishing Credible Sources
  13. Promoting Lifelong Learning
    - Utilizing eBooks for Skill Development

- Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
  - Interactive and Gamified eBooks

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