# Large amplitude vibrations in molecules

*Internal Rotation and Inversion: An Introduction to Large Amplitude Motions in Molecules.* By D. G. Lister, J. N. Macdonald and N. L. Owen. Pp.246. (Academic: London and New York, 1978.) £11.50.

LARGE amplitude low frequency vibrations comprise a somewhat specialised topic within the subject of molecular vibration–rotation spectroscopy. However, they comprise a topic of particular interest for a number of reasons and are thus a deserving subject for a specialist text. The interest arises because these vibrations represent motions along the valleys in the molecular potential energy surface, so that they are of especial interest in the molecular dynamics of conformational changes and chemical reactions. Also, the experimental data on the energy levels of low frequency vibrations may be extensive (in contrast to the usual situation for other vibrations), and the theory by which they are related to the potential energy surface does not fall into the usual pattern of vibrational theory. Thus, in principle a book on this subject might be of interest to a wide range of chemical physicists.

This book starts with an introductory chapter on the concept of large amplitude vibrations, with many examples, and diagrams of sections of potential energy surfaces. Chapter 2 deals with basic theory, chapter 3 gives a cursory account of experimental methods (microwave, infrared, Raman and NMR spectroscopy, and electron diffraction), chapter 4 reviews *ab initio* and semi-empirical potential surface calculations, and the remaining five chapters discuss particular examples of large amplitude vibration in more detail—essentially internal rotation, inversion and ring puckering vibrations, and conformational motions in macromolecules.

Although the physical ideas are well presented, the authors have attempted to write a book which is not too taxing in mathematical theory and quantum mechanics. Sympathetic as I am to this ambition, the serious student has to face up to the theory, for indeed the relationship of experimental spectra to potential surface should be the unifying theme of the subject. Thus, I found the book weak in the very area where I feel it should be strong. The theory is loose where the student wants rigour; the material is badly organised; some important topics are not mentioned and others are discussed twice in different places without any apparent correlation. As examples of these defects: on p23 "transpose" should read "conjugate transpose"; equation (2.45) on p42 lacks a factor $h^2/2I$; different methods of solving the Mathieu equation are discussed on p42 and p111 without any cross reference or comments to help the reader; and the effects of inversion on rotational constants are also discussed twice, on p58 and p70, again without cross reference (why is a first power term in $x$ included on p70 and not on p58?), although one might reasonably have expected to find this discussion in chapter 7 or chapter 8. Many passages give me the impression that they will be of little help to a student who does not already know the subject, and of even less help to the student who does; as examples of this, consider the page about Van Vleck transformations (p25–26), or the four pages about gas electron diffraction (p81–84). The important topic of the symmetry of nonrigid molecules, developed in the past ten years by Longuet-Higgens, Hougen, Bunker, and others, does not seem to be mentioned anywhere in the book. Quasi-linear molecules are an important class of molecules with large-amplitude vibration that are not discussed.

The book has its good points; one of them is indeed the subject itself! But in today's sophisticated and competitive world of specialist scientific textbooks, I feel that it has not been written with the care and attention to detail that are necessary for success.

**Ian M. Mills**

*Ian M. Mills is Professor of Chemistry at the University of Reading, UK.*

# Thin films and the electronics industry

*Thin Films: Interdiffusion and Reactions.* Edited by J. M. Poate, K. N. Tu and J. W. Mayer. Pp.578. (Wiley: New York and Chichester, UK, 1978.) £25.

MANY reasons are advanced to explain why our scientific and inventive abilities in the physical sciences are frequently not realised in industry. One good reason is the failure by scientists and industry alike to treat product design and manufacturing processes as vital technologies which must develop their own specialised sciences if inventiveness is to be fulfilled in the market. We all know, without effect, that this common neglect stems from our history when science developed rapidly and modern industry was founded, both occurring almost independently. This unsatisfactory division rooted in the scientist of independent means and the practical manufacturer has lead to the notions that the study of how one makes things and how they perform is too close to common work to be regarded as suitable activities for trained minds; and in any case such investment is wasteful. Only during the last War did scientists effectively join with industry to develop expertise; but so quickly did we slip back that we now seem to have no defence against another crisis—that of market competition.

If one doubts the validity of these comments then it is only necessary to read recent views of the decision of the National Enterprise Board to enter the microprocessor field. Expert opinion on this relates to financial investment problems, preference for licencing overseas know-how, industrial need for microprocessors regardless of dependence on supply, and the novelty of the electronics and their social effects. Nowhere have I found any mention of what must be done to found a satisfactory industry in the UK for the manufacture of large scale integrated electronics. For example, who supplies the process plant? A new area of electronics cannot be established without the association of scientists and engineers developing production and product know-how and training skilled workers, that is, if the enterprise is to be more than a manufacturing unit with off-shore control of every aspect of its activities.

The book under review dealing with problems encountered in making and operating solid-state devices illustrates what must be done to establish such an industry. It also shows how US companies are able to create the industrial science needed for the purpose at hand. There remarks are not intended to be disparaging of the work done by R & D scientists in solid-state laboratories in the UK but to point up the effects of inadequate R&D funding in an industry which once enjoyed a position next to the US in the world league.

The book's editors have experience of the subjects treated from research in their laboratories. Dr Poate, a one-time Harwell Fellow, is now with Bell Laboratories; Dr Tu is a specialist in solid-state diffusion at the IBM Thomas J. Watson Research Center; and Professor Mayer is concerned with ion/atom collision effects at the California Institute of Technology. Their contributions are supplemented by others from research colleagues and members