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## International Union of Crystallography

Acta Cryst. (1985). B41, 205

## Availability of deposited atomic coordinates from the Cambridge Crystallographic Data Centre

Over the past few years an increasing number of journals have adopted the policy of depositing atomic coordinates relating to organic and metalorganic structures with the Cambridge Crystallographic Data Centre (CCDC). It appears that there has been some misunderstanding about accessing such deposited data and concern about its availability to interested scientists. This note by the CCDC is intended to clarify the situation.

Deposited data are available on request from the CCDC and a note to this effect is included in each publication which involves deposited data. The CCDC responds promptly, and free of charge, to each request either by sending a photocopy of the original deposited tables or, if the structure has already been checked and entered into the Structural Database, by sending a computer listing of the data together with other key information and a plot of the structure.

Deposited data incorporated in the Structural Database are also available by accessing tape copies of the Database distributed through National Affiliated Centres and individual laboratories in the following countries: Australia, Austria, Belgium, Brazil, Canada, CSSR, Denmark, Finland, France, Federal Republic of Germany, Hungary, India, Israel, Italy, Japan, The Netherlands, New Zealand, Norway, Saudi Arabia, South Africa, Switzerland, UK, USA and USSR. However, as indicated above, deposited data can be obtained directly from the CCDC. Deposited data are thus available worldwide independent of the distribution and currency of the Structural Database.

## **Book Reviews**

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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Smectic liquid crystals: textures and structures. By G. W. GRAY and J. W. GOODBY. Pp. xxvi+162. Glasgow: Leonard Hill, 1984. Price £46.00.

Smectics (from the greek  $\sigma\mu\eta\gamma\mu\alpha$ : soap, rubber) are layered systems, like soap itself and many stearate, laurate, etc..., salts in water, or phospholipids in water. The mention of these chemical species is sufficient to indicate the importance of these modifications of condensed matter in applied sciences and biophysics. But, as elements of a set of materials displaying a remarkable polymorphism, these are also of intrinsic fundamental interest. This book deals with a second group of smectics, made of pure organic compounds, with elongated molecules having a rigid central aromatic part, and more or less flexible moieties of various chemical natures. Fundamental problems in chemistry, molecular and structural properties, ..., are more at hand with this second group, whose study has been developed considerably in the last 15 years without showing any sign of unrest up to now, on the contrary. The same molecules are also at the origin of other liquid-crystalline mesophases, like nematic, cholesteric and 'blue' phases. The authors of this monograph, after a short introductory chapter which contains a reasonable bibliographical account of nematic, cholesteric and blue phases (also with a bibliography concerning mesophases made of plate-like molecules), turn to a detailed and systematic description of smectic polymorphism, each of the first nine chapters being devoted to one of the known smectic phases (in the alphabetic order of the terminology, viz A, B, ..., I); chapter 10 is an update of the previous chapters which, but for a few exceptions, deal with results obtained before 1982. Chapter 10 contains, in particular, a brief account of: the hexatic phase, which has proved important as a concrete example of two-dimensional melting; antiphase behaviour in the bilayered structures of nitro and cyano compounds, where the existence of a longitudinal dipole brings new interesting ordering features; and ferroelectric phases of chiral molecules, much studied today for display devices; it ends with a detailed and useful table of the structural properties of smectic phases. The whole text is completed by a beautiful series of 124 colour optical micrographs of the typical textures displayed by the various smectic modifications.

Gray and Goodby are chemists and have played an important role in the synthesis of new liquid-crystalline molecules and in the discovery of liquid-crystalline phases. With any new material of these types the standard methods of characterization used by the chemists are (1) inspection of the textures using optical polarizing microscopy, (2) a study of the possible miscibility of the new material with a reference material: if miscibility prevails, the two materials are of the same type, (3) DTA and DSC measurements. X-ray diffraction patterns and the investigation of molecular properties by NMR or quasi-elastic neutron scattering are of course more involved methods, which should bring the final touch to this kind of study, but there are good (and fundamental) reasons why the simpler methods could be sufficient and even possibly more rewarding. Each chapter contains an account of the structure of typical representative materials of the corresponding modification, often attended by an historical recall of the difficulties the scientists met in reaching an agreement on the modification, sometimes completed by a short review of the theoretical background. Then identification and classification methods are described, in the following order: microscopic textures, miscibility studies, X-ray diffraction, DSC and DTA.

This book comes at a very suitable time; there is still very little activity in the study of the physical properties of all the new modifications discovered in the last 10 years: the physicists have been struck with admiration by this abundance of riches and have not yet reacted appropriately. Therefore this book will be read with profit not only by newcomers in the field, but also by more enlightened scientists. I hope it is successful. I would like however, especially for newcomers, to stress a few essential ideas whose importance in my opinion is underrated by the authors: for example, I think it must be said that the characterization of modifications by the use of textures is not a method which rests on a purely descriptive approach, but possesses a very elaborate scientific background: the physics of defects. Defects which are present in a given texture relate to the history of the sample (thermal history, annealings, recovery processes, if phase transitions are quickly or slowly passed across, ...). Metallurgists have a lot to teach us in this area. Defects depend also on the symmetry group of the modification, in a very fundamental way. The authors seem to ignore the fact that the molecular structure of the three essential liquid-crystalline modifications (nematic, cholesteric, smectic) were discovered by Georges Friedel (see his remarkable 1922 paper in Annales de Physique) by the sole inspection of defects in the polarizing microscope, long before X-ray diffraction patterns proved he was right. The epistemological value of this success cannot be underestimated. In that perspective, it is important to know that focal conic domains are genuine defects in smectic phases only if the layers are able to glide one upon the other without change of free energy: as far as I know, this is true only for SmA, SmC and hexatic SmB phase (I value this notation, SmX, over the notation used by the authors,  $S_X$ where a capital letter is inconveniently used as subscript). In the SmA and SmC cases, the focal conics are able to reach huge sizes (millions of layers involved), although the theory predicts an algebraic decay of the layer-layer correlation, a result that the authors emphasize perhaps too strongly in view of this undeniable experimental fact. In all cases where the layers do not glide easily, focal domains must be paramorphotic. Intermediary cases must be interesting to study. In any respect, such considerations should be known by the polarizing-microscope practitioner, as well as others (amongst very many: it should be noted that the fan texture of SmA phases is closely similar to the usual texture of hexagonal discotic phases), for the sake of

efficiency. From the point of view of the scientific content of observations, the older book of Demus and Richter, written before many new smectic phases had blossomed, and also illustrated with many photographic plates, remains irreplaceable, thanks to its introduction on defects. Similarly, since the authors deal so much with miscibility criteria, it would have been valuable for the book to contain a few phase diagrams, which would have recalled to the reader in a very easy way that miscibility criteria are not universal, and that areas of perfect miscibility are separated by biphasic spindles or miscibility gaps. On the whole, this work remains, however, an excellent introduction to a very promising field, and should stimulate studies in molecular and submacroscopic properties of smectic modifications. Phase transition temperature data are often lacking in the text as well as the temperatures at which the pictures have been taken. It would be useful if such data could appear in a second edition.

M. KLÉMAN

Laboratoire de Physique des Solides (CNRS) Université de Paris-Sud Bâtiment 510 91405-Orsay France

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The rare earths in modern science and technology. Vol. 3. Edited by G. J. MCCARTHY, H. B. SILBER and J. J. RHYNE. Pp. xxiii+588. New York: Plenum, 1982. Price US \$59.50.

This volume is the third of a new series recording the proceedings of the annual conferences taking place in the USA on rare-earth research. Like its predecessors this is a voluminous book, reproducing the text of some 120 research papers given at the 1981 meeting. The previous volume, relating to the 1980 meeting, was reviewed by Caro [Acta Cryst. (1982), B38, 1685].

The spectrum of varied phenomena in which rare-earth elements and their compounds are involved, in physics and chemistry, is impressive. We find spectroscopic and magnetic studies, of course, but also research results in bioinorganic chemistry, electrochemistry, phase equilibria and transitions, organometallic chemistry and coordination chemistry, and many other varieties of work represented here. In these widely ranging reports, the structures of crystals as such are merely an occasional minor component but throughout there is recurring recourse to structural investigations of many kinds, in which X-ray and neutron diffraction (usually in polycrystalline mode) frequently figure.

This is emphatically not a textbook on the rare earths. It is simply yet another volume of conference proceedings, useful to those working specifically in this field.

J. H. ROBERTSON

School of Chemistry University of Leeds Leeds LS2 9JT England