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D:C-friedo-B':A'-neo-Gammacer-9(11)-ene: erratum. By HELMUT W. SCHMALLE and OTTO H. JARCHOW. *Mineralogisch-Petrographisches Institut der Universität Hamburg, Grindelallee 48, D-2000 Hamburg 13, Federal Republic of Germany* and BJÖRN M. HAUSEN, *Universitäts-Hautklinik Hamburg Eppendorf, Martinistrasse 52, D-2000 Hamburg 20, Federal Republic of Germany*

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Abstract

There is a typographical error in the *Abstract* of the paper by Schmale, Jarchow & Hausen [*Acta Cryst.* (1980). B36,

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2450–2453]. The correct value of the cell constant b is 10.751 (7) Å.

All relevant information is given in the *Abstract*.

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Book Reviews

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Atlas of molecular structures in biology. Vol. 2. Haemoglobin and myoglobin. By G. FERMI and M. F. PERUTZ. Pp. vi + 104. Oxford Univ. Press, 1981. Price £20.00.

The amount of structural information about a particular protein can be very large, and is usually scattered over numerous publications over a period of many years (more than two decades for hemoglobin and myoglobin). Furthermore, conventional journals are frequently poorly equipped for the representation of three-dimensional data. Hence, D. C. Phillips and F. M. Richards initiated the publication of a series of atlases. The first publication concerned itself with the relatively small ribonuclease molecule [Richards & Wyckoff (1973). *Ribonuclease-S*. Oxford Univ. Press]. It was an original and useful experiment in various representations of a three-dimensional complex structure. The present volume is an extension of this approach to the far more complex oligomeric hemoglobin molecule. The *Atlas* is well bound with connected wire loops in order to permit the pages to fall easily onto a flat viewing surface. About half of the material is text and tables while the other half is figures. The principal three-dimensional representations are red–green stereo diagrams (a pair of filters is supplied with the book). These diagrams can show large surfaces in three dimensions as their size is not limited by normal eye separation. Furthermore, viewing is unaccompanied by eye strain as is usual with conventional left–right stereo diagrams. The major technical problem is the difficulty of finding a suitable blue–green ink to match with the green eye filter, causing a faint blue image in the vicinity of the three-dimensional image. The diagrams in the Fermi and Perutz *Atlas* are no exception. Furthermore, some of the diagrams have been

printed rather faintly (e.g. D2 and D3) causing a different kind of eye strain. However, the diagrams in this book, which are drawn with meticulous care for detail and clarity, are far superior to the usual journal representations and, short of a model, the best available method for illustrating a very complex molecule.

The *Atlas* is divided into two parts. The first, written by Giulio Fermi, is a true atlas. The text explains easily and clearly the differences between the relaxed, *R* (liganded hemes) and tensed, *T* (unliganded) states of hemoglobin. The alteration of the quaternary structure between the *R* and *T* states controls the function of hemoglobin. In contrast, myoglobin, a monomer, can only have a single state. In hemoglobin, the four active subunits (two α and two β chains) communicate with each other by altering the association between subunits. The approximately 0.4 Å movement of the iron in and out of the plane of the heme group causes small alterations in the subunit tertiary structures which are amplified onto a large 18° rotation of the $\alpha_1\beta_1$ dimer relative to the $\alpha_2\beta_2$ dimer. Hence, the study of the heme interactions with the globin and the subunit interactions are central to an understanding of how hemoglobin works. The subunit interactions in hemoglobin are shown in tabular form (Figs. 8, 9) for both the *R* and *T* states and are illustrated with side chains (D18–D27). One wonders why the authors did not experiment with some 'space-filling' views to augment the study of subunit interactions. The heme environments are illustrated for the met (liganded) and deoxy (unliganded) forms of myoglobin and the α and β chains of hemoglobin. The species used for illustration are sperm whale for myoglobin and primarily human adult deoxyhemoglobin and horse methemoglobin. No diagrams are provided showing the superposition of these structures on each other, but the differences are carefully described in the text and in tables. In addition, there is a

wealth of information in tabular and figure form with excellent text which can be readily appreciated by anybody. Nearly all the data have been deposited in the Brookhaven Protein Data Bank and can, therefore, be treated to further and different analyses by any interested person.

The second part of the *Atlas* was prepared by Max Perutz. Here he probes the molecular mechanism by comparing the structure and properties of abnormal and fetal hemoglobins with normal (A) hemoglobin. Fortunately for the study of hemoglobin, they are still a fairly rapidly evolving family of proteins. Hence, the rate of accepted point mutations is relatively high and the number of abnormal hemoglobulins found in the human population is appreciable. Well over 30 such hemoglobulins have been studied in some detail. The best known example is that of sickle-cell hemoglobin (S) where a glutamine on the β chain in position 3 on α -helix A changes to a valine causing the formation of destructive crystalline fibers in the red cells of venous blood. Such single alterations give precise probes into the molecular properties causing change of oxygen affinity, alteration in the cooperativity between subunits and the Bohr effect. These abnormalities are discussed by Perutz in relation to the structure illustrated in the first part of the *Atlas*. There are shown a number of black and white on grey electron density maps as experimental evidence of the structural information. Unfortunately, the difference electron density maps on pages 92 and 93 are not accompanied, like the others, by explanatory diagrams. Some of the descriptions of the structural alterations (e.g. the heme is more upright or inclined) are dependent on the view of the observer and require unavailable information of a standard model. This section is, however, a fantastic compendium of information and its mostly successful analysis in terms of the properties of hemoglobin is a tremendous achievement.

An alternative approach to the study of hemoglobin is the analysis of globins from widely different species. This has been the procedure of Love and co-workers as well as a number of other laboratories around the world. Unlike the abnormal human hemoglobins, these structures are not isomorphous with oxy or deoxy human hemoglobin A and the amino acid differences are numerous rather than in a well defined and specific position. Consequently, the differences in properties and structure are on a much larger scale. Recognition of this alternative approach is given on page 102 of the *Atlas* where Table 16 gives invariant residues. The treatment here is brief indeed, and does not balance the detail in the first 101 pages. No doubt, however, data on the other globins will be the topic of future editions by the appropriate authors.

The Fermi-Perutz *Atlas* is far more than a substantial work on hemoglobin and myoglobin. It is a magnificent example of how a complex molecule has been investigated. The analysis of the regulation of subunit interactions is appropriate not only to all cooperative oligomeric enzymes but, for instance, bears also on the assembly of viruses where small switches provided by cations or the binding of phosphates (in the form of nucleic acids) can substantially alter the preferred subunit associations.

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Ionophores and their structures. By MAX DOBLER. Pp. 379. New York, London: John Wiley, 1981. Price £42.50.

Ionophores are defined as 'substances which promote the transfer of ions from an aqueous medium into a hydrophobic phase'. These include naturally occurring peptide and depsipeptide ionophores and their synthetic analogues, the macrolide antibiotics, naturally occurring carboxylic acid ionophores and synthetic ionophores, such as macrocyclic 'crown' polyethers, and 'cryptates'.

The early chapters summarize the biophysical and the chemical investigations of the compounds mainly with respect to their complexing ability with alkali-metal and alkaline-earth-metal cations. There is an extensive table of formation constants and selectivity sequences. Use of chiral complexes for separation of racemates is also mentioned. All is compressed into 38 pages which give a good independent survey.

The main part of the book is a compendium of the results of X-ray crystal structure analysis on the ionophore molecules and their complexes. These are drawn as stereo pairs by the excellent program *PLUTO* of the Cambridge Crystallographic Data Centre. The author has obtained unpublished coordinates, not only from those files, but also from original authors (and, in fact, the book has already saved me from writing a letter). Appendices show displayed structural formulae with the numbering and the orthogonal coordinates of the unique molecules in Å enabling the reader to carry out further geometrical calculations. Many of these calculations have already been done by the author who provides tables of dimensions of interest, such as torsion angles in complexed and uncomplexed molecules and important bond lengths. In the text he discusses the significance of the results and is particularly good in critical appraisal of apparent contradictions in the literature. The nature of the book probably owes something to the author's experience of having to determine the structure of a potassium valinomycin complex himself to obtain the coordinates years after a preliminary communication from another laboratory.

Coverage of the literature is reasonably complete to 1979. The price is not unreasonable in view of the large number of illustrations.

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X-ray diffraction by disordered and ordered systems. By D. W. L. HUKINS. Pp. ix + 164. Oxford: Pergamon, 1981. Price US\$28.75.

The aim of this little book is to show how the X-ray scattering phenomenon is used to achieve structural data on