SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1993). **B49**, 145

Structures of cubic and orthorhombic phases of acetylene by single-crystal neutron diffraction. Erratum.

By R. K. McMullan and Å. Kvick, *Chemistry Department, Brookhaven National Laboratory, Upton, NY* 11973, *USA*, and P. Popelier, *Department of Chemistry, University of Antwerp (UIA), Universiteitsplein* 1, *B*-2610 *Wilrijk, Belgium*

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Abstract

An error in technical editing is corrected. In the paper by McMullan, Kvick & Popelier [*Acta Cryst.* (1992), **B48**, 726–731], the crystal classes of acetylene (C_2H_2) at 131 and 141 K and deuteroacetylene (C_2D_2) at 143 and 15 K are given incorrectly. The correct assignments are: acetylene is cubic at 131 and 141 K, and deuteroacetylene is cubic at 143 K and orthorhombic at 15 K.

All relevant information is given in the *Abstract*.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, *USA). As far as practicable, books will be reviewed in a country different from that of publication.*

Acta Cryst. (1993). **B49**, 145–146

Accurate molecular structures, their determination and importance. (IUCr Monograph on Crystallography No. 1.)

Edited by A. Domenicano and I. Hargittai. Pp. xii + 590. Oxford University Press, 1992. Price £60.00. ISBN 0-198-55556-3.

Molecular structure can be described at many levels of exactitude and definiteness, from squiggles drawn on the back of an old envelope to the exquisite precision in equilibrium geometry and vibrational behaviour attainable by modern spectroscopic and diffraction methods as well as, at least for small molecules, by quantum-mechanical calculations. For some purposes, only the overall topology of a molecule may be of interest - is the methyl group *cis* or *trans* to the hydrogen at the ring junction? For other purposes, we may need a careful examination of factors influencing random and systematic errors implicit in particular experimental techniques - is an apparent shortening by 0.006 Å of some bond distance in a crystal structure study compared with a gas-phase study due to systematic error in one or the other type of measurement or is it a real effect that calls for explanation in terms of crystal packing forces? Questions of this type abound. Especially now that small differences in equilibrium bond distances in related molecules can be interpreted in terms of differences in chemical reactivity, answers to such questions can even have some practical utility. This book provides authoritative chapters dealing with the possibilities and limitations of structural studies at the molecular level where the emphasis is on the attainment of maximum possible accuracy.

A general historical introduction (Angelo Gavezzotti and the late Massimo Simonetta, 13 pp.) is followed by a discussion of the concept of the molecular potential energy surface (Kozo Kuchitsu, 33 pp.). Then come three chapters on the determination of gas-phase molecular structures; by microwave spectroscopy (Bouke P. van Eijck, 18 pp.), infrared spectroscopy (Georges Graner, 30 pp.) and electron diffraction (István Hargittai, 31 pp.).

The following six chapters, beginning with a general introduction to X-ray crystallography (Jenny P. Glusker and Aldo Domenicano, 44 pp.), deal with the methods, results and possibilities of accurate crystal structure analysis and constitute what is essentially a modern textbook on the subject. A chapter by Paul Seiler (29 pp.) examines the main sources of error in measuring Bragg intensities and shows how they should be corrected for (or, better still, avoided) in accurate work. Two chapters deal with the analysis of atomic motion in crystals, the first (Kenneth N. Trueblood, 21 pp.) taking us up to the limitations of the mean-field model, the second (Carlo M. Gramaccioli, 17 pp.) beyond them into lattice-dynamical interpretations. The characteristically thorough and critical chapter by the late Fred L. Hirshfeld (33 pp.) should be

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declared compulsory reading for crystallographers wishing to make electron-density studies based on diffraction measurements. The most accurate available crystal structures, with respect to both molecular geometry and motional description, come from low-temperature (*e.g.* 15 K) neutron diffraction analyses. George A. Jeffrey (29 pp.) shows how results from such analyses compare with those from *ab initio* computations and how subtle differences provide information about how molecules may be deformed by crystal field effects.

It is not so well known that precise structural parameters for small symmetric molecules can be derived from NMR coupling constants measured in oriented solvents, *i.e.* liquid crystals. This topic is discussed in a chapter by Peter Diehl (23 pp.), who shows that structural parameters obtained in this way are quite comparable with those obtained by other spectroscopic techniques or by gas-phase electron diffraction.

The next three chapters deal with computational methods. James E. Boggs (14 pp.) describes the calculation of equilibrium geometries and vibrational constants by molecular orbital calculations; results for small symmetric molecules are comparable to those from good experiments, and the range of application of the method will surely be extended as even bigger and better computers become available. Norman L. Allinger has a chapter (19 pp.) on the development and present status of molecular mechanics and Frank H. Allen has one (24 pp.) on the retrieval and analysis of molecular structural information from the Cambridge Structural Database.

The last six chapters deal with applications in the border areas between structural and mechanistic chemistry. Georges Wipff and Stéphane Boudon (33 pp.) discuss mainly the structural expression of electron delocalization and other stereoelectronic effects; Valeria Ferretti, Katharina C. Dubler-Steudle and Hans-Beat Bürgi (25 pp.) explain how structure correlations can be used to derive information about chemical reaction pathways and energy surfaces for chemical reactions; Aldo Domenicano (32 pp.) reviews structural substituent effects in benzene derivatives; Joel Bernstein (29 pp.) examines the effect of the crystal environment on molecular structure - comparison of molecules in different polymorphic modifications can be most informative. Jeremy K. Burdett swings expertly between experiment and theory in his chapter (32 pp.) where he describes how accurate structure determination has illuminated several problems of inorganic chemistry - the role of agostic hydrogen atoms in transition-metal chemistry is one. And, finally, Vincenzo G. Albano and Dario Braga (25 pp.) discuss structural variability in metal cluster compounds.

This book has been a long time in the making. Its starting point was a set of lecture notes prepared by the instructors at an International School of Crystallography course entitled 'Static and Dynamic Implications of Precise Structural Information' held at the Ettore Majorana Centre for Scientific Culture at Erice, Sicily, in 1985. The seven-year interval between the Erice school and publication of the book has not been in vain. The authors of the various chapters and the editors have evidently put in a great deal of work, with the result that most contributions have gained in thoroughness, perspective, and clarity. In pleasing contrast to most other multi-authored books of this kind, effective editing has reduced repetitious overlap between the various contributions to a minimum; in its place, extensive cross referencing connects related material in different chapters. In addition, the material has been kept reasonably up to date with many references to the post-1985 literature. The overall result is that the original lecture notes have been transformed into an important book which will remain the standard work for teachers, students and researchers for many years to come.

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Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Structure reports for 1984. Vol. 51B. Parts 1 and 2. Organic compounds. Edited by GEORGE FERGUSON. Pp. vi + 2094. Dordrecht: Kluwer Academic Publishers, 1992. Price Dfl 680.00. ISBN 0-7923-1758-0. The present volume continues the aim of *Structure Reports* to present critical accounts of all crystallographic structure determinations. 724 pages are devoted to organic compounds, 256 pages to main-group compounds and 977 pages to transition-metal compounds. Subject, formula and author indices are provided.

Quasicrystals, networks and molecules of fivefold symmetry. Edited by I. HARGITTAI. Pp. xiii + 314. New York, Weinheim and Cambridge: VCH Publishers, 1990. Price £55.00. ISBN 089573723X. A review of this book, by J. H. Robertson, has been published in the January 1993 issue of *Acta Crystallographica*, Section A, pages 214-215.

Introductory solid-state physics. By H. P. MYERS. Pp. xi + 546. London: Taylor and Francis, 1990. Price (paper) £18.00. ISBN 0850667615. A review of this book, by B. J. Hickey, has been published in the January 1993 issue of *Acta Crystallographica*, Section A, page 215.