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*

(*Received* 5 *November* 1992)

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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