

Acta Cryst. (1977), **B33**, 316

On the structure of (Cr_5Al_8) 26R. A correction. By J. W. VISSER, *Technisch Physische Dienst TNO-TH, PO Box 155, Delft, The Netherlands*

(Received 26 August 1976; accepted 12 September 1976)

An error in *Strukturbericht* (1940, 5, 11) and Pearson [*A Handbook of Lattice Spacings and Structures of Metals and Alloys* (1967), Vol. 2, p. 111. Oxford: Pergamon Press] is pointed out with the help of the original data.

The structure of Cr_5Al_8 was determined by Bradley & Lu (1937), by analogy with the structure of Cu_5Zn_8 . The latter compound has a cubic body-centred unit cell with $a = 8.86 \text{ \AA}$, whereas Cr_5Al_8 can be described on a body-centred rhombohedral unit cell with $a = 9.0508 \text{ \AA}$ and $\alpha = 89.273^\circ$. In order to indicate the close similarity between the two structures, Bradley & Lu give their final atomic parameters in terms of this body-centred rhombohedral cell. Unfor-

tunately they also state in their paper the primitive unit cell (rhombohedral, $R3m$, $a = 7.805$, $\alpha = 109.127^\circ$) without giving the atomic parameters in terms of this cell. As a result, the reports in both *Strukturbericht* (1940, 5, 11) and Pearson (1967) give the small unit cell with the atomic parameters of the large (body-centred) cell.

A transformation from the rhombohedral body-centred cell to the rhombohedral primitive cell is $[-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} / \frac{1}{2}, -\frac{1}{2}, \frac{1}{2} / \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}]$. The new atomic parameters can then be calculated from the old ones from $X_{\text{new}} = Y_{\text{old}} + Z_{\text{old}}$, $Y_n = Z_o + X_o$, $Z_n = X_o + Y_o$, resulting in the parameter list of Table 1. The new parameters were used to calculate the interatomic distances, which agreed well with those given by Bradley & Lu.

Table 1. *Structure of (Cr_5Al_8) 26R: space group $R3m$, $a = 7.8051 \text{ \AA}$, $\alpha = 109.217^\circ$, $Z = 2$*

		x	y	z
1 Cr in 1(a)	x,x,x	0.194		
3 Cr in 3(b)	x,x,z	0.003		0.794
3 Cr in 3(b)	x,x,z	0.998		0.340
3 Cr in 3(b)	x,x,z	0.355		0.006
1 Al in 1(a)	x,x,x	0.672		
3 Al in 3(b)	x,x,z	0.654		0.012
3 Al in 3(b)	x,x,z	0.349		0.582
3 Al in 3(b)	x,x,z	0.722		0.356
6 Al in 6(c)	x,y,z	0.033	0.288	0.661

References

- BRADLEY, A. J. & LU, S. S. (1937). *Z. Kristallogr.* **96**, 20–37.
 PEARSON, W. B. (1967). *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, Vol. 2, p. 111. Oxford: Pergamon Press.

International Union of Crystallography

Eleventh General Assembly and International Congress of Crystallography

By invitation of the Polish Academy of Sciences the Eleventh General Assembly and International Congress of Crystallography will be held in Warsaw, Poland, 3–12 August 1978.

The arrangement of the scientific programme will in general be similar to that of the Tenth Congress held in Amsterdam 1975. There will be General Lectures, Scientific Sessions on topics of interest for today's crystallography, chemistry and solid state physics, Poster Sessions, Open Sessions of Commissions of the Union and *ad hoc* meetings. Participants will be invited to submit abstracts of recent work on crystallographic subjects. Upon acceptance, these contributions will be printed in the book of abstracts of the Congress. For oral presentation in the formal scientific sessions or for the poster sessions, a selection will be made from the papers lying within the range of the Congress topics. The *ad hoc* meetings are intended mainly to encourage free discussion.

An exhibition of non-commercial equipment and of photographs and drawings of crystallographic interest will be held during the Congress. More detailed information can be

obtained from the Organizing Committee. A commercial exhibition will be organized in which manufacturers and distributors of equipment related to crystallographic research may display their products. Further information may be obtained from the Organizing Committee. For the accompanying members, a choice of tours will be offered. The details of this programme and the social programme will be published in the *First Circular*. Travel information may be obtained from the offices of Polish Airlines LOT and Polish Travel Office ORBIS.

Professor J. Auleytner is Chairman of the Organizing Committee. Other members are Dr J. Leciejewicz (Vice-Chairman), Dr Z. Gałdecki and Dr T. Warminiński (Secretary). Correspondence should be addressed to the secretariat at the following address:

Eleventh International Congress of Crystallography
 Polish Academy of Sciences
 Institute of Physics
 IF PAN SL-1
 Al. Lotników 32/46, Pawilon 9
 02-668 Warszawa
 Poland.

Telephone: Warszawa 43 60 34. Telex: 81 24 64.

Further details of the Congress, including arrangements for registration, accommodation, scientific visits, *etc.*, will be published in the *First Circular*, which will be distributed in the second half of 1977. Persons interested in receiving the *First Circular* are requested to complete an application card

and return it to the Organizing Committee before 1 June 1977. Application cards may be obtained from the Secretaries of the National Committees for Crystallography or from the Organizing Committee. Please bring this announcement to the notice of your colleagues.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

European Crystallographic Committee

The European crystallographers, through the European Crystallographic Committee, invite colleagues in developing countries to join in co-operation schemes. The purpose of the co-operation is to exchange information, teaching material and staff, to share facilities such as data, collecting apparatus, to assist potential buyers of equipment to contact the main suppliers and to set up joint research programmes.

Active crystallographers and/or departments with crystallography groups, who are interested in such a co-operation scheme are invited to contact either Professor Dr D. Feil, Chemical Physics Laboratory, Twente University of Technology, PO Box 217, Enschede, The Netherlands, or the President of the European Crystallographic Committee: Dr O. Kennard, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England.

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.

Molecular structure – the physical approach. By J. C. D. BRAND and J. S. SPEAKMAN. 2nd edition revised by J. C. SPEAKMAN and J. K. TYLER. Pp. vi + 367, Figs. 120, Tables 69. London: Arnold, 1975. Price £11.00, paper £5.50.

I accepted the task of reviewing this bright small book with great pleasure because of the debt I have to its first edition. The first edition has been of great help to me (as a textbook) in teaching the methods of determination of molecular structure in the physical chemistry courses at my University. In my teaching experience this book has certainly been successful in its purposes – giving, in a general and sufficiently concise way (but not for this less rigorous), the theoretical fundamentals of the methods for molecular structure determination.

This second edition has maintained the same philosophy as the first. On the one hand it gives a sufficiently sound explanation of the physical principles on which the experimental methods are based; on the other, it helps the researcher who uses these methods to realize not only why they are employed but also that they offer many more possibilities than those with which he is accustomed to be content.

The book certainly achieves its aim and is particularly instructive for students who need a first general account of the subject before going more deeply into it, possibly in successive specialist courses.

After an introductory chapter on the concept of the molecule and on the range of physical methods available for studying molecular structures, the concept of symmetry is tackled from both the spectroscopic (isolated molecules) and crystallographic (molecules packed in crystals) points of view. Group theory is employed in a simple and elegant way; of course, only point groups are dealt with by group theory as the treatment of space groups would be too cumbersome and outside the aims of this book.

That part more strictly devoted to molecular spectroscopy takes up the following seven chapters and represents about 60% of the whole work. After a chapter on the fundamentals of quantum mechanics and another giving an introductory survey of spectroscopic methods, pure rotation, vibration, Raman and nuclear resonance spectra are considered successively. Well chosen examples are used to clarify the concepts and their importance in the various applications.

Only two chapters are devoted to diffraction methods, one