



Fig. 1. A representation of the crystal structure of TMCC viewed along the c axis. Chains formed by face-sharing of octahedrally coordinated cadmium-chloride ion, $-\text{Cd}-\text{Cl}_3-\text{Cd}-$, are parallel to the a axis at the origin; $[\text{N}(\text{CH}_3)_4]^+$ ions are located between these chains in a disordered manner.

parameters for this case are given in Table 1. The observed and calculated structure factors obtained with these parameters are given in Table 2. The crystal structure of TMCC as viewed along the c axis is represented in Fig. 1.

The slight trigonal elongation (Table 3) of the octahedron about the cadmium ion is very similar to that observed in TMMC (84.09 and 95.91°). The longer Cd-Cl separation compared with Mn-Cl (2.560 Å) results in a slight elongation of the cell dimension along the c axis; this increased separation between the chloride ions along the chain allows the $[\text{N}(\text{CH}_3)_4]^+$ ions to fit closer to the chains, resulting in a slightly smaller a axis (for TMMC, $a_0 = 9.1510$ and $c_0 = 6.4940$ Å). Even though an improvement would be

Table 3. Interatomic separations and angles in TMCC

(a) Involving chemically bonded atoms (for labeling, see Fig. 1):			
Cd-Cl(1)	2.644 (1) Å	Cl(1)-Cd-Cl(2)	83.91 (3)°
N-C(1)	1.34 (3)	Cl(1)-Cd-Cl(3)	96.09 (3)
N-C(2)	1.47 (3)	C(1)-N-C(2)	101 (2)
		C(2)-N-C(3)	116 (1)
(b) Involving near-neighbor contact separations within chain and $[\text{N}(\text{CH}_3)_4]^+$ ion:			
Cl(1)-Cl(2)	3.535 (2) Å	C(1)-C(2)	2.17 (4) Å
Cl(1)-Cl(3)	3.933 (1)	C(2)-C(3)	2.50 (2)
(c) Involving near-neighbor contact separation between chain and/or $[\text{N}(\text{CH}_3)_4]^+$ ions:			
Cl(2)-C(3)	3.54 (2) Å	C(1)-C(4)	4.28 (3) Å
Cl(1)-C(2)	3.74 (2)	C(2)-C(4)	4.28 (5)
Cl(1)-Cl(4)	3.84 (4)		
Cl(1)-C(5)	3.83 (2)		

obtained for comparison of the carbon-carbon bond lengths with standard accepted values, those listed in Table 3 were not corrected for 'in phase' motion (Busing & Levy, 1964), because it is felt that the approximation of the model used (statistically disordered $[\text{N}(\text{CH}_3)_4]^+$ ions with atoms undergoing anisotropic harmonic thermal motion) is inadequate to describe the smeared electron density map mentioned above.

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References

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Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

Molecular structures and dimensions. Vol. 1. Bibliography 1935-69. General organic crystal structures. Edited by OLGA KENNARD and DAVID G. WATSON. Pp. xxiii + 413. Utrecht: Oosthoek's, 1970. Price f32 (\$10, £3.90), library copy: f45 (\$14, £5.40).

Molecular structures and dimensions. Vol. 2. Bibliography 1935-69. Complexes and organometallic structures. Edited by OLGA KENNARD and DAVID G. WATSON. Pp. xxiii + 364. Utrecht: Oosthoek's, 1970. Price f27 (\$8.50, £3.30), library copy: f35 (\$11, £4.30).

These two volumes are precisely what their titles claim, a list of titles and authors of some 4000 crystal structures

published between 1935 and 1 January 1969, together with some 500 of the structure analyses published during 1969. The bibliography refers to carbon-containing compounds, but omits what the authors describe as 'purely inorganic substances such as inorganic carbides, carbonyls, carbonates, cyanides and thiocyanates'. The omission of cyanides and thiocyanates is inconvenient but the omission of metal carbonyls I find quite extraordinary.

The criteria of a good bibliography must be its comprehensiveness within its declared criteria, its ease of use and its accuracy. On the first of these counts I must compliment the authors on their work. In some six months of use I have been able to fault the bibliography only once and that with a paper of obscure title in an obscure journal. Unfortunately the editors decided to have an indefinite termination date for the present section and I hope that the

500 structures already listed for 1969 will reappear in the 1969/70 section which has already gone to press, otherwise self-evident difficulties may arise.

The bibliography is, I find, easier to use when looking for purely organic molecules than it is for metal complexes. The compounds are listed by fairly narrow classes: for example, aliphatic amines, phenols, ethers, benzoquinones, *etc.* in Vol. 1, and by rather more broadly defined ligand types, *e.g.* metal π -complexes (cyclopentadiene)metal complexes (nitrogen ligand) *etc.* in Vol. 2. Within any particular class the listing is according to empirical formula by carbon content. The system tends to break down if it is necessary to search for a variety of complexes of a given metal atom. To help counteract this disadvantage the authors have included a metal index, but one which merely catalogues those structures containing a particular metal. For the limited size of the bibliography at the present time this system is just bearable, but it will, I believe, become a grave disadvantage when, say, another ten years have passed by.

Maximum use of computers has been made in the compilation and typesetting of the volumes. On the whole the process has been very accurate, though I do observe the authors J. Ame, R. Che and M. So.

On the whole I feel I must congratulate Drs Kennard and Watson on what will prove to be, I am sure, a publication invaluable to all researchers interested in molecular structure.

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Introduction to molecular spectroscopy. By E. F. M. BRITAIN, W. O. GEORGE and C. H. J. WELLS. Pp. xi+387. New York: Academic Press, 1971. Price £6.00.

This is a book intended primarily for undergraduate chemists, and it claims to provide comprehensive coverage of the subject for this purpose. In addition to an Introduction, wherein the usual basic theoretical relations are developed, there are chapters on Electronic, Vibrational, Nuclear Magnetic Resonance, and Mass Spectrometry.

A bold attempt is made in the introductory chapter to provide the reader with a sufficiency of group theory to

tackle the symmetry properties of the direct product representations involved in transition moment integrals. Though neatly done, this must be unsuccessful with the complete beginner at whom the treatment clearly is aimed. A satisfactory working knowledge of the essentials of group theory simply cannot be transmitted in less than six pages of text. It is probably virtually inevitable that the massive condensation of material involved here should have led to vagueness in places (is the student not likely to be puzzled by *irreducible representations* and their *characters* when presented with no reference at all to matrices?), and misstatements in others (*e.g.* 'the wave function in the ground state is always totally symmetric' – given in a completely general way). However, to compensate for this, the Introduction contains a particularly clear and useful section on the significance of wave functions.

Within the more specialized chapters the authors have quite successfully summarized the essential features of the selected techniques, and even provide sets of experiments which serve to illustrate applications and some aspects of the theory. The condensation again has occasionally led to oversimplification, as in the treatment of *d-d* electronic transitions where only the *d¹* and *d⁹* configurations are considered, and even then no mention is made of Jahn-Teller effects. However, to include in a single book (of 387 pages in all, including a useful index) such an immense range of material, from basic theory through to considerable detail on experimental procedures, instrument evaluation, *etc.* and retain essential clarity represents a major achievement of this work. The student already acquainted with the elements of group theory and wave mechanics will find it a useful introductory survey. The layout of experiments suggests use of the book also as a laboratory manual, though it is doubtful whether it will in practice find much use as such.

A mixture of S. I. and non-S. I. units is used throughout the book, the authors evidently being unconvinced that the cm^{-1} and eV, among others, are on their way out. Since more specialized books are more likely to be of use to advanced students, and the price of this one is beyond the reach of most beginners, it is difficult to commend this book to any individual reader in spite of its many good features. It will doubtless be found useful in large library collections.

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