Molecular Structures and Dimensions

3

Bibliography 1969-71

Organic and Organometallic Crystal Structures

Edited by
Olga Kennard and David G Watson

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University Chemical Laboratory, Cambridge

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Introduction

This volume is the third classified bibliography of organic and organometallic crystal structures prepared by the Crystallographic Data Centre, University Chemical Laboratory, Cambridge, and published jointly with the International Union of Crystallography.

The two previous volumes covered the period 1935–1969. Volume 1 dealt with general organic structures and Volume 2 with complexes, organometals and organometalloids, whose structures were analysed by X-ray or neutron diffraction methods. Entries were arranged in chemical classes, with classes 1–59 in volume 1 and 60–86 in volume 2.

The present volume covers classes 1–86 and provides references to compounds whose structures were reported in the literature during 1969–1971. A number of structures published prior to 1969 and omitted from the previous volumes are also included. The arrangement of entries is identical with the first two volumes and the reader is referred to the Introduction in these volumes for a description of the practical use of the bibliography.

There are three indexes in the present volume: formula, transition metal and author indexes. All are cumulative for the period 1935–1971 and give references to entries in Vols. 1–3.

The bibliography and indexes are prepared, checked and printed by computer techniques described in the previous volumes. Magnetic tapes of the three volumes are available and anyone interested should contact the Centre for further details.

In order to improve the cut-off date 9 journals, covering approximately 78% of the crystallographic literature, were scanned directly.

The source for the remaining references was the abstracting journal Bulletin Signalétique, published by the Centre National de la Recherche Scientifique, Paris, France. Abstracts appear in the Bulletin Signalétique some 6–10 months following the publication in the primary journals. Included in the present volume are the

conference proceedings of the American Crystallographic Association for the years 1967 to 1971 and the papers presented at the 8th International Congress of Crystallography, August 1969. Thus the cut-off dates for Vol. 3 can be summarised as follows:

Acta Cryst. (B), part 5, 1971
J. Chem. Soc. (A), part 11, 1971
J. Chem. Soc. (B), part 6, 1971
J. Chem. Soc. (C), part 6, 1971
J. Chem. Soc. (D), part 13, 1971
J. Amer. Chem. Soc., part 6, 1971
Acta Chem. Scand., part 1, 1971
Inorg. Chem., part 6, 1971
Tetrahedron Letters, part 12, 1971
Other Journals: complete for 1969,
partially scanned for 1970

The work of the Crystallographic Data Centre is supported by the Office for Scientific and Technical Information, Department of Education and Science, as part of the British contribution to international data activities.

We are greatly indebted to readers who have notified us of mistakes and omissions in Vols. 1 and 2. We have tried to improve our check procedures in the light of experience with the production of the previous volumes, but errors must inevitably still be present. We would appreciate readers alerting us to these and any suggestions for future improvements.

Cambridge July 1971 *Olga Kennard and David G. Watson*

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The production of this bibliography was a collaborative effort by members of the Crystallographic Data Centre: Drs F.H. Allen, N.W. Isaacs, W.D.S. Motherwell, R.C. Pettersen, P.J. Roberts, W.G. Town, Miss E. Ross, Mrs M. Smith, Mrs K.A.M. Watson, Mrs S.M. Weeds and Miss H. Young.

Dr Town has made the principal contribution to the development of the overall program system required for the regular updating, maintenance and processing of the bibliographic file.

Mrs Weeds was responsible for literature searches, primary abstracting and problems relating to chemical nomenclature. In the latter activity she was assisted by Mrs Smith.

Mrs Watson has been in charge of the encoding of information and the registration and checking of new material. In the secretarial work of documentation she has been assisted by Miss Young.

Drs Allen, Isaacs, Motherwell, Pettersen and Roberts have contributed to the literature scanning and proof-reading of the final listings.

The work of the Centre was guided by members of the OSTI Scientific Advisory Committee: Professor J.W. Linnett, FRS, Dr M.F. Lynch, Dr F.W. Matthews, Professor D.C. Phillips, FRS, Professor M.R. Truter and Professor A.J.C. Wilson, FRS (chairman).

We are grateful to the Medical Research Council for allowing a member of their External Scientific Staff (O. Kennard) to participate in this work.

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Our task was greatly facilitated by the excellent organisation of the Centre National de la Recherche Scientifique, which provided

copies of most of the references listed in the bibliography. Dr R.S. Cahn and the Nomenclature Division of the Chemical Abstracts Service have helped with questions of nomenclature.

We have used the IBM 360/44 computer at the Institute of Theoretical Astronomy and we were greatly helped by both the programming staff and operators. We are grateful to INSPEC (Information Service in Physics, Electrotechnology and Computers & Control) and especially to Mr P. Simmons for the use of their computer typesetting programs, which they specially modified for our purposes.

The bibliography was prepared in parallel with the organic section of "Crystal Data" (National Bureau of Standards, Washington D.C., USA) and both publications were strengthened through this collaboration.

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List of Classes

Note—classes marked with an asterisk (*) contain no entries in Volume 3.

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CH_2O_2 , CH_3NO
For complete entry see 60.3

1.C **Barium hydrogen oxalate dihydrate**
$C_2H_2O_4$, $C_2O_4^{2-}$, Ba^{2+} , $2H_2O$
For complete entry see 2.5

1.1 **N - Bromoacetamide**
C_2H_4BrNO
R.J.Dubey *Acta Cryst. (B)*, **27,** 23, 1971

1.2 **Acetic acid (at 5 ° C)**
$C_2H_4O_2$
I.Nahringbauer *Acta Chem. Scand.*, **24,** 453, 1970

1.3 **Acetic acid (at −190 ° C)**
$C_2H_4O_2$
I.Nahringbauer *Acta Chem. Scand.*, **24,** 453, 1970

1.4 **Acetic acid (neutron study, at −140 ° C)**
$C_2H_4O_2$
P.-G.Jonsson *Acta Cryst. (B)*, **27,** 893, 1971

1.C **Ammonium acetate - acetic acid complex (at −56 ° C)**
$C_2H_4O_2$, $C_2H_3O_2^-$, H_4N^+
For complete entry see 2.11

1.5 **Glycolic acid**
$C_2H_4O_3$
W.P.Pijper *Acta Cryst. (B)*, **27,** 344, 1971

1.6 **Glycolic acid (neutron study)**
$C_2H_4O_3$
R.D.Ellison, C.K.Johnson, H.A.Levy *Acta Cryst. (B)*, **27,** 333, 1971

1.7 **Acetamide hemihydrobromide**
$C_2H_6NO^+$, C_2H_5NO , Br^-
J.Weimann, H.Gillier-Pandraud, N.Thoai, C.Beaute
Bull. Soc. Chim. Fr., 2147, 1969

1.8 **Fluoromalonic acid**
$C_3H_3FO_4$
G.Roelofsen, J.A.Kanters, J.Kroon, J.A.Vliegenthart
Acta Cryst. (B), **27**, 702, 1971

1.9 **Dichloromalonamide**
$C_3H_4Cl_2N_2O_2$
J.A.Lerbscher, K.V.Krishna Rao, J.Trotter *J. Chem. Soc. (A)*, 1505, 1971

1.10 **Cyanoacetamide**
$C_3H_4N_2O$
P.C.Chieh, J.Trotter *J. Chem. Soc. (A)*, 184, 1970
Also classified in 7

1.11 **Malonamide**
$C_3H_6N_2O_2$
P.C.Chieh, E.Subramanian, J.Trotter *J. Chem. Soc. (A)*, 179, 1970

1.12 **N - Methyl - chloroacetamide**
C_3H_7ClNO
Y.Koyama, T.Shimanouchi, Y.Iitaka *Acta Cryst. (B)*, **27**, 940, 1971

1.C **3,5 - Di - iodo - L - thyronine - N - methylacetamide complex**
C_3H_7NO , $C_{15}H_{13}I_2NO_4$
For complete entry see 60.43

1.13 **Acetylene dicarboxylic acid**
$C_4H_2O_4$
H.Irngartinger, L.Leiserowitz, G.M.J.Schmidt *J. Chem. Soc. (B)*, 497, 1970

1.14 **Monochloroacetic anhydride**
$C_4H_4Cl_2O_3$
A.J.de Kok, C.Romers *Rec. Trav. Chim. Pays-Bas*, **88**, 625, 1969

1.C **Potassium hydrogen fumarate**
$C_4H_4O_4$, $2C_4H_3O_4^-$, $2K^+$
For complete entry see 2.18

1.15 **Fumaramic acid**
$C_4H_5NO_3$
F.L.Hirshfeld *Acta Cryst. (B)*, **27**, 769, 1971

1.16 **Trinitrobutyric acid**
$C_4H_5N_3O_8$
C.M.Bock
Amer. Cryst. Assoc., Abstr. Papers (Winter Meeting), 41, 1970
Also classified in 10

1.17 **(–) - 2 - Bromosuccinamic acid (absolute configuration)**
$C_4H_6BrNO_3$
Y.Murakami, Y.Iitaka *Chem. Pharm. Bull., Jap.*, **17**, 2397, 1969

1.18 **Methylmalonic acid**
$C_4H_6O_4$
J.L.Derissen *Acta Cryst. (B),* **26,** 901, 1970

1.19 **(+) - Tartaric acid (absolute configuration)**
$C_4H_6O_6$
H.Hope, U.de la Camp *Nature,* **221,** 54, 1969

1.C **Betaine hydrochloride**
$C_5H_{12}NO_2^+$, Cl^-
For complete entry see 48.17

1.C ***Dipotassium cis* - aconitate**
$C_6H_4O_6^{2-}$, $2K^+$
For complete entry see 2.20

1.20 **racemic - Thiodilactic acid**
$C_6H_{10}O_4S$
E.Martuscelli, L.Mazzarella, R.Palumbo, C.Pedone
Ric. Sci., **39,** 573, 1969
Also classified in 11

1.21 **Dilactylamide (optically active)**
$C_6H_{12}N_2O_2$
E.Martuscelli, L.Mazzarella, R.Palumbo, C.Pedone
Ric. Sci., **39,** 573, 1969

1.C **Carbamoylcholine bromide**
$C_6H_{15}N_2O_2^+$, Br^-
For complete entry see 3.24

1.22 **racemic - 3 - Bromo - 4,4 - dihydroxypimelic acid dilactone**
$C_7H_7BrO_4$
L.Brehm *Acta Chem. Scand.*, **24,** 3480, 1970
Also classified in 38

1.C **4 - Methylcarbamoylcholine bromide**
$C_7H_{17}N_2O_2^+$, Br^-
For complete entry see 3.33

1.23 **Butane - 1,2,3,4 - tetracarboxylic dianhydride**
$C_8H_6O_6$
R.Nagao, F.Marumo, Y.Saito, T.Asahara
Acta Cryst. (B), **27,** 569, 1971

1.24 **trans - trans - Dimethyl - 2,5 - dichloro - 2,4 - hexadienedioate**
$C_8H_8Cl_2O_4$
H.M.Einspahr, J.Donohue
Amer. Cryst. Assoc., Abstr. Papers (Summer Meeting), 91, 1968

1.25 **p - Chlorocinnamide**
C_9H_8ClNO
D.Rabinovich *J. Chem. Soc. (A)*, 2361, 1969

1.C **p - Coumaric acid**
$C_9H_8O_3$
For complete entry see 17.5

1.C **Hippuric acid**
$C_9H_9NO_3$
For complete entry see 13.9

1.26 **Azelamide (at −140 ° C)**
$C_9H_{18}N_2O_2$
M.Hospital *Acta Cryst. (B)*, **27**, 484, 1971

1.27 **Azelamide (at 120 ° C)**
$C_9H_{18}N_2O_2$
M.Hospital *Acta Cryst. (B)*, **27**, 484, 1971

1.28 **Azelamide**
$C_9H_{18}N_2O_2$
M.Hospital *Acta Cryst. (B)*, **27**, 484, 1971

1.29 **p - Bromophenacyl dichloroacetate**
$C_{10}H_7BrCl_2O_3$
J.C.Calabrese, A.T.McPhail, G.A.Sim *J. Chem. Soc. (B)*, 285, 1970

1.30 **p - Bromophenacyl difluoroacetate**
$C_{10}H_7BrF_2O_3$
J.C.Calabrese, A.T.McPhail, G.A.Sim *J. Chem. Soc. (B)*, 285, 1970

1.31 **2,2,4,4 - Tetramethyladipic acid**
$C_{10}H_{18}O_4$
E.Benedetti, C.Pedone, G.Allegra *Macromolecules*, **3**, 16, 1970

1.32 **β - Phenylglutaric acid**
$C_{11}H_{12}O_4$
G.Avitabile, P.Ganis, E.Martuscelli *J. Chem. Soc. (D)*, 1362, 1970

1.C **3 - Benzylamino - 4 - hydroxypent - 2 - enoic acid lactone hydrobromide (optically active)**
$C_{12}H_{16}NO_2^+$, Br^-
For complete entry see 3.43

1.C **racemic - 3 - Benzylamino - 4 - hydroxypentanoic acid lactone hydrochloride**
$C_{12}H_{16}NO_2^+$, Cl^-
For complete entry see 3.44

1.C **4 - Phenylcarbamoyl choline bromide**
$C_{12}H_{19}N_2O_2^+$, Br^-
For complete entry see 3.45

1.C **5,6 - Dimethyl - 4 - phenylcarbamoylcholine bromide**
$C_{14}H_{23}N_2O_2^+$, Br^-
For complete entry see 3.50

1.C **Succinylcholine iodide**
$C_{14}H_{30}N_2O_4^{2+}$, $2I^-$
For complete entry see 3.51

1.33 α - **Benzamido - trans - cinnamic acid**
$C_{16}H_{13}NO_3$
K.Brocklehurst, R.P.Bywater, R.A.Palmer, R.Patrick
J. Chem. Soc. (D), 632, 1971
Also classified in 13

1.34 **3 - p - Tolylthio - trans - cinnamic acid**
$C_{16}H_{14}O_2S$
F.S.Stephens *J. Chem. Soc. (A),* 1843, 1970
Also classified in 11

1.35 **Dodecane - 1,12 - dioic acid di - 1,1′ - monoglyceride (β form)**
$C_{18}H_{34}O_8$
K.Larsson, L.Sjostrom *Ark. Kemi,* **30,** 1, 1969

1.36 **Stearic acid (form C)**
$C_{18}H_{36}O_2$
V.Malta, G.Celotti, R.Zannetti, A.F.Martelli *J. Chem. Soc. (B),* 548, 1971

1.37 **Methyl stearate (orthorhombic form)**
$C_{19}H_{38}O_2$
C.H.MacGillavry, M.Wolthius-Spuy *Acta Cryst. (B),* **26,** 645, 1970

1.38 **trans,trans - Di - p - methoxybenzylidene - succinic anhydride (orthorhombic form)**
trans,trans - Di - p - anisylidene fulgide
$C_{20}H_{16}O_5$
M.D.Cohen, H.W.Kaufman, D.Sinnreich, G.M.J.Schmidt
J. Chem. Soc. (B), 1035, 1970
Also classified in 17

1.39 **11 - Bromoundecanoic acid 1,3 - diglyceride**
$C_{25}H_{46}Br_2O_5$
A.Hybl, D.Dorset *Acta Cryst. (B),* **27,** 977, 1971

ALIPHATIC CARBOXYLIC ACID SALTS (AMMONIUM, IA, IIA METALS)

2.C **DL - Tryptophan formate**
CHO_2^- , $C_{11}H_{13}N_2O_2^+$
For complete entry see 48.42

2.1 **Strontium formate dihydrate**
$2CHO_2^-$, Sr^{2+} , $2H_2O$
K.Osaki *Ann. Rep. Scient. Works Fac. Sci. Osaka,* **6,** 13, 1958

2.2 **Potassium oxalate monohydrate (neutron study)**
$C_2O_4^{2-}$, $2K^+$, H_2O
A.Sequeira, S.Srikanta, R.Chidambaram *Acta Cryst. (B),* **26,** 77, 1970

2.3 **Lithium oxalate monoperhydrate**
$C_2O_4^{2-}$, $2Li^+$, H_2O_2
B.F.Pedersen *Acta Chem. Scand.,* **23,** 1871, 1969

2.4 **Ammonium oxalate monoperhydrate**
$C_2O_4^{2-}$, $2H_4N^+$, H_2O_2
B.F.Pedersen *Acta Chem. Scand.,* **23,** 342, 1969

2.5 **Barium hydrogen oxalate dihydrate**
$C_2O_4^{2-}$, $C_2H_2O_4$, Ba^{2+} , $2H_2O$
Y.Dusausoy, J.Protas, J.C.Mutin, G.Watelle
Acta Cryst. (B), **26,** 1567, 1970
Residue 2 classified in 1

2.6 **Potassium hydrogen oxalate**
$C_2HO_4^-$, K^+
H.Einspahr, R.E.Marsh, J.Donohue
Amer. Cryst. Assoc., Abstr. Papers (Winter Meeting), 36, 1971

2.7 **Lithium hydrogen oxalate monohydrate**
$C_2HO_4^-$, Li^+ , H_2O
H.Follner *Z. Anorg. Allg. Chem.,* **373,** 198, 1970

2.8 **Sodium hydrogen oxalate monohydrate**
$C_2HO_4^-$, Na^+ , H_2O
H.Follner, J.A.Kanters, J.Kroon *Naturwissenschaften,* **57,** 193, 1970