Molecular Structures and Dimensions

5

Bibliography 1972-73

Organic and Organometallic Crystal Structures

Edited by
Olga Kennard, David G Watson and
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University Chemical Laboratory, Cambridge

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Introduction

This volume is the fifth 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 first four volumes covered the years 1935–1972. The present volume provides references principally to compounds whose structures were reported in the literature during 1972–1973. A few structures published prior to 1972 and omitted from the previous volumes are also included. The arrangement of entries in the 86 chemical classes is identical with the previous volumes and the reader is referred to the Introduction in Vol. 1 or Vol. 2 for a description of the practical use of the bibliography.

There are three cumulative indexes in the present volume: formula, transition metal and author indexes. All three cover the period 1935–1973 and give references to entries in Vols. 1–5.

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

In the present volume we have continued the special arrangement for literature search with the Centre National de la Recherche Scientifique, Paris, France. Under this arrangement reprints of papers containing crystallographic data are sent directly to the Crystallographic Data Centre, Cambridge, at the same time as they are sent out to abstractors preparing material for the Bulletin Signalétique. As a result this material is incorporated in our files at an estimated 3–6 months following the publication in the primary journals, and even before the appearance of the abstract in the Bulletin Signalétique.

In addition to the above arrangement, 10 journals, covering approximately 78% of the crystallographic literature, are scanned

directly in Cambridge. The cut-off dates for Volume 5 can be summarised as follows:

Acta Cryst. (B), part 6, page 1364, 1973
J. Chem. Soc. Dalton, part 13, page 1420, 1973
J. Chem. Soc. Perkin II, part 8, page 1200, 1973
J. Chem. Soc. Chem. Comm., part 14, page 508, 1973
J. Amer. Chem. Soc., part 11, page 3824, 1973
Acta Chem. Scand., part 3, page 1113, 1973
Inorganic Chemistry, part 6, page 1464, 1973
Tetrahedron Letters, part 28, page 2660, 1973
J. Cryst. Mol. Struct., part 2, page 123, 1973
Cryst. Struct. Comm., part 2, page 374, 1973
Other Journals: complete for 1971
ca. 95% complete for 1972
ca. 30% complete for 1973

The following Conference Abstracts were included in Vol. 5:

Conference Proceedings of the American Crystallographic Association, Summer 1972, Winter 1973.

The Stockholm Symposium on the Structure of Biological Molecules, July 1973.

First European Crystallography Meeting, Bordeaux, France, September 1973.

Joint meeting of the Italian and Jugoslav Crystallographic Association, Trieste, Jugoslavia, June 1973.

We would like to draw our readers' attention to the first of the numeric tables which has just been published in this series: Vol. A1 'Interatomic Distances 1960–1965, Organic and Organometallic Crystal Structures'. The new volume is a continuation of the 'Tables of Interatomic Distances and Configuration in Molecules and Ions' (Chemical Society Special Publications No. 11, London 1958; No. 18, London 1965) which covered the literature until the end of 1959. Volume A1 contains numeric data, including bond lengths, bond angles and torsion angles for about 1,300 structures analysed by X-ray and neutron diffraction. Numeric volumes for the later years are also planned.

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. 1–4. We have attempted to modify our procedures and are at present considering further changes including changes in the contents of forthcoming volumes. We would be grateful to readers for any suggestions on how these volumes could be further improved.

Cambridge November 1973

Olga Kennard, David G. Watson, William G. Town

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The production of this bibliography was a collaborative effort by members of the Crystallographic Data Centre: Dr F. H. Allen, Mrs A. Doubleday, Dr W. D. S. Motherwell, Mrs K. Watson, Miss C. P. Way and Mrs S. Weeds.

Mrs Weeds was responsible for literature searches, primary abstracting and problems relating to chemical nomenclature.

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 C. P. Way.

Drs Allen and Motherwell have contributed to the literature scanning, primary editing and proof reading of the final listings.

The work of the Centre was guided by members of the OSTI Scientific Advisory Committee: Professor D. W. J. Cruickshank, Mr O. S. Mills, Dr P. Owston, 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.

We thank the University of Cambridge for the provision of accommodation in the University Chemical Laboratory and for the administration of the OSTI grant.

Our task was greatly facilitated by the excellent organisation of the Centre National de la Recherche Scientifique. We are especially grateful to Madam C. Degen of the CNRS who was responsible for the improved literature searches referred to in the Introduction.

We have used the IBM 370/165 computer of the University of Cambridge 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 volume of 'Crystal Data' (National Bureau of Standards, Washington D.C., USA). The third edition was published in the summer of 1972 and both publications were strengthened by this collaboration.

Contents

List of Classes

ALIPHATIC CARBOXYLIC ACID DERIVATIVES

1.C **Oxalic acid - acetamide complex**
$C_2H_2O_4$, C_2H_5NO
For complete entry see 60.1

1.C **Furamide - oxalic acid complex**
$C_2H_2O_4$, $2C_5H_5NO_2$
For complete entry see 60.3

1.1 **Difluoroacetamide**
$C_2H_3F_2NO$
D.O.Hughes, R.W.H.Small *Acta Cryst. (B),* **28,** 2520, 1972

1.2 **Acetic acid - phosphoric acid complex**
$C_2H_4O_2$, H_3O_4P
P.-G.Jonsson *Acta Chem. Scand.*, **26,** 1599, 1972

1.3 **Acetic acid - phosphoric acid complex (neutron study)**
$C_2H_4O_2$, H_3O_4P
P.-G.Jonsson *Acta Chem. Scand.*, **26,** 1599, 1972

1.C **Oxalic acid - acetamide complex**
C_2H_5NO , $C_2H_2O_4$
For complete entry see 60.1

1.C **Potassium tri - hydrogen di - malonate (neutron study)**
$C_3H_3O_4^-$, $C_3H_4O_4$, K^+
For complete entry see 2.14

1.C **3,5 - Di - iodo - L - thyronine - N - methylacetamide complex (absolute configuration)**
C_3H_7NO , $C_{15}H_{13}INO_4$
For complete entry see 60.28

1.4 **2 - (N - Nitrosomethylamino)acetamide**
$C_3H_7N_3O_2$
L.K.Templeton, D.H.Templeton, A.Zalkin *Acta Cryst. (B),* **29,** 50, 1973
Also classified in 9, 10

1.C **Malonic dihydrazide monohydrate**
$C_3H_8N_4O_2$, H_2O
For complete entry see 9.1

1.C **Potassium hydrogen acetylenedicarboxylate (α form)**
$C_4HO_4^-$, K^+
For complete entry see 2.15

1.C **Rubidium hydrogen acetylenedicarboxylate (β form,data set I)**
$C_4HO_4^-$, Rb^+
For complete entry see 2.16

1.C **Rubidium hydrogen acetylenedicarboxylate (β form,data set II)**
$C_4HO_4^-$, Rb^+
For complete entry see 2.17

1.5 **Acetylene dicarboxylic acid (for high - angle refinement see Jungk and Schmidt,Chem.Ber.,105,2607,1972)**
$C_4H_2O_4$
V.Benghiat, L.Leiserowitz, G.M.J.Schmidt *J. C. S. Perkin II,* 1769, 1972

1.6 **But - 3 - ynoic acid**
$C_4H_4O_2$
V.Benghiat, L.Leiserowitz *J. C. S. Perkin II,* 1772, 1972

1.7 **Tetrolic acid (α form)**
$C_4H_4O_2$
V.Benghiat, L.Leiserowitz *J. C. S. Perkin II,* 1763, 1972

1.8 **Tetrolic acid (β form)**
$C_4H_4O_2$
V.Benghiat, L.Leiserowitz *J. C. S. Perkin II,* 1763, 1972

1.9 **Maleic acid**
$C_4H_4O_4$
M.N.G.James, G.J.B.Williams
Amer. Cryst. Assoc., Abstr. Papers (Winter Meeting), 85, 1973

1.C **Potassium hydrogen fumarate**
$C_4H_4O_4$, $2C_4H_3O_4^-$, $2K^+$
For complete entry see 2.19

1.10 **(–) - Chlorosuccinic acid (absolute configuration)**
$C_4H_5ClO_4$
L.Kryger, S.E.Rasmussen, J.Danielsen *Acta Chem. Scand.*, **26,** 2339, 1972

1.11 **Fumaramic acid**
$C_4H_5NO_3$
V.Benghiat, H.W.Kaufman, L.Leiserowitz, G.M.J.Schmidt
J. C. S. Perkin II, 1758, 1972

1.C **Benzamide - succinic acid complex**
$C_4H_6O_4$, $2C_7H_7NO$
For complete entry see 60.9

1.C γ - **Aminocrotonic acid hydrobromide**
$C_4H_8NO_2^+$, Br^-
For complete entry see 48.12

1.C γ - **Aminocrotonic acid hydrobromide**
$C_4H_8NO_2^+$, Br^-
For complete entry see 48.13

1.C γ - **Aminobutyric acid**
$C_4H_9NO_2$
For complete entry see 48.18

1.C γ - **Amino** - β - **hydroxybutyric acid**
$C_4H_9NO_3$
For complete entry see 48.19

1.C γ - **Aminobutyric acid hydrochloride**
$C_4H_{10}NO_2^+$, Cl^-
For complete entry see 48.25

1.12 β - **Chloroglutaric acid anhydride**
$C_5H_5ClO_3$
F.J.Koer, A.J.de Kok, C.Romers
Rec. Trav. Chim. Pays-Bas, **91,** 691, 1972
Also classified in 38

1.13 **Mesaconic acid**
$C_5H_6O_4$
M.P.Gupta, S.R.P.Yadav *Acta Cryst. (B),* **28,** 2682, 1972

1.14 **N - (2,2,2 - Trinitro - isopropyl) - chloroacetamide**
$C_5H_7ClN_4O_7$
B.V.Gidaspov, N.V.Grigor'eva, N.V.Margolis, G.V.Makarenko, E.I.Popov, V.F.Selivanov *Zh. Strukt. Khim.*, **12,** 1117, 1971

1.15 **DL - Methylsuccinic acid**
$C_5H_8O_4$
Y.Schouwstra *Acta Cryst. (B),* **29,** 1, 1973

1.16 γ - **Guanidinobutyric acid hydrobromide**
$C_5H_{12}N_3O_2^+$, Br^-
K.-I.Tomita *Tetrahedron Letters,* 2587, 1971
Residue 1 also classified in 8

1.C **Potassium dihydrogen trans - aconitate**
$C_6H_5O_6^-$, K^+
For complete entry see 2.28

1.17 **trans,trans - Muconic acid**
$C_6H_6O_4$
J.Bernstein, L.Leiserowitz *Israel J. Chem.*, **10,** 601, 1972

1.18 **N - Methyl - citraconamic acid**
$C_6H_9NO_3$
F.H.Allen, O.Kennard *Cryst. Struct. Comm.*, **2,** 145, 1973

1.19 **meso - Tartaric acid dimethyl ester**
$C_6H_{10}O_6$
J.Kroon, J.A.Kanters *Acta Cryst. (B),* **29,** 1278, 1973

1.20 ε - **Amino - n - caproic acid**
$C_6H_{13}NO_2$
A.Takenaka, T.Yamamoto, K.-I.Yamasaki, A.Furusaki, I.Nitta
Kwansei Gakuin Univ. Ann. Studies, **18,** 127, 1969
Also classified in 48

1.21 **N - Methyl - dipropylacetamide**
$C_7H_{19}NO$
C.Cohen-Addad, A.Grand, J.Lajzerowicz *Eur. Cryst. Meeting,* 1973

1.22 **Dimethyl - (dimethylaminomethylene) - malonate**
$C_8H_{13}NO_4$
U.Shmueli, H.Shanan-Atidi, H.Horwitz, Y.Shvo
J. C. S. Perkin II, 657, 1973
Also classified in 3

1.C **3 - Acetoxypropyl - trimethylammonium bromide**
$C_8H_{18}NO_2^+$, Br^-
For complete entry see 3.17

1.23 β - **Chloro - cis - cinnamic acid**
$C_9H_7ClO_2$
S.E.Filippakis, L.Leiserowitz, D.Rabinovich, G.M.J.Schmidt
J. C. S. Perkin II, 1750, 1972

1.24 β - **Chloro - trans - cinnamic acid**
$C_9H_7ClO_2$
S.E.Filippakis, L.Leiserowitz, D.Rabinovich, G.M.J.Schmidt
J. C. S. Perkin II, 1750, 1972

1.25 **N - Methyl - di - n - propylacetamide**
$C_9H_{19}NO$
A.Grand, C.Cohen-Addad *Acta Cryst. (B),* **29,** 1149, 1973

1.26 β - **Methyl - cis - cinnamic acid**
$C_{10}H_{10}O_2$
S.E.Filippakis, L.Leiserowitz, D.Rabinovich, G.M.J.Schmidt
J. C. S. Perkin II, 1750, 1972

1.C **Ammonium 2,3 - di - isopropyl - maleamate**
$C_{10}H_{16}NO_3^-$, H_4N^+
For complete entry see 2.30

1.27 **Ethylenediaminetetra - acetic acid (β form)**
$C_{10}H_{16}N_2O_8$
M.F.C.Ladd, D.C.Povey *J. Cryst. Mol. Struct.*, **3,** 15, 1973
Also classified in 3

1.28 **9 - Keto - trans - 2 - decenoic acid**
$C_{10}H_{16}O_3$
D.T.Cromer, A.C.Larson *Acta Cryst. (B),* **28,** 2128, 1972

1.C **N - Acetyl - DL - pseudo - leucyl - dimethylamide**
$C_{10}H_{20}N_2O_2$
For complete entry see 48.62

1.29 **N,N′ - Diethyladipamide**
$C_{10}H_{20}N_2O_2$
E.Benedetti, M.R.Ciajolo, P.Corradini *Europ. Polymer J.*, **9,** 101, 1973

1.30 **N - Propyl - dipropylacetamide**
$C_{11}H_{23}NO$
C.Cohen-Addad, A.Grand, J.Lajzerowicz *Eur. Cryst. Meeting,* 1973

1.31 **Tripropylacetamide**
$C_{11}H_{23}NO$
C.Cohen-Addad, A.Grand, J.Lajzerowicz *Eur. Cryst. Meeting,* 1973

1.C **bis(11 - Ammonio - undecanoic acid) tetrachlorocuprate**
$2C_{11}H_{24}NO_2^+$, Cl_4Cu^{2-}
For complete entry see 3.21

1.32 **N,N - Diethyl - phenylacetamide**
$C_{12}H_{17}NO$
G.Allegra, G.Avitabile, E.Benedetti, M.R.Ciajolo, P.Corradini, P.Ganis, M.Goodman, A.Immirzi, C.Pedone *Acta Cryst. (A),* **28,** S13, 1972

1.33 **Ethyl p - chloro - α - cyano - β - methyl - cis - cinnamate**
$C_{13}H_{12}ClNO_2$
T.Higuchi, W.Nagai, K.Nakatsu, T.Miwa, A.Shimada
Israel J. Chem., **10,** 221, 1972
Also classified in 19

1.34 **N - Propyl - tripropylacetamide**
$C_{14}H_{29}NO$
C.Cohen-Addad, A.Grand, J.Lajzerowicz *Eur. Cryst. Meeting,* 1973

1.C **3 - (p - Bromophenyl)propionic acid cyclohexanone - cyanohydrin ester**
$C_{16}H_{18}BrNO_2$
For complete entry see 21.10

1.C **Mycophenolic acid**
$C_{17}H_{20}O_6$
For complete entry see 17.19