# Molecular Structures and Dimensions

6

## Bibliography 1973-74

## Organic and Organometallic Crystal Structures

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# Introduction

This volume is the sixth 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 five volumes covered the years 1935–1973. The present volume provides references principally to compounds whose structures were reported in the literature during 1973–1974. A few structures published prior to 1973 and omitted from the previous volumes are also included.

In this volume an attempt has been made to standardise the classification system for classes 1–59 and a precedence ordering of classes 1–86 has been introduced. Details are presented on pp. xiii.

There are three cumulative indexes in the present volume: formula, transition metal and author indexes. All three cover the period 1935–1974 and give references to entries in Vols. 1–6.

The bibliography and indexes were prepared, checked and printed by computer techniques described in the previous volumes. Magnetic tapes of the six 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.

In addition to the above arrangement, 11 journals, covering approximately 78% of the crystallographic literature, are scanned

directly in Cambridge. The cut-off dates for Volume 6 can be summarised as follows:

Acta Cryst. (B), part 7, page 1880, 1974
J. Chem. Soc. Dalton, part 13, page 1424, 1974
J. Chem. Soc. Perkin II, part 8, page 946, 1974
J. Chem. Soc. Chem. Comm., part 15, page 627, 1974
J. Amer. Chem. Soc., part 12, page 4041, 1974
Acta Chem. Scand. (A), part 3, page 347, 1974
Acta Chem. Scand. (B), part 4, page 381, 1974
Inorganic Chemistry, part 7, page 1791, 1974
Tetrahedron Letters, part 29, page 2545, 1974
J. Cryst. Mol. Struct., part 2, page 97, 1974
Cryst. Struct. Comm., part 3, page 569, 1974
Other Journals: complete for 1972
ca. 95% complete for 1973
ca. 30% complete for 1974

The following Conference Abstracts were included in Vol. 6:

Conference Proceedings of the American Crystallographic Association, Summer 1973, Spring 1974.

We would like to draw our readers' attention to the first of the numeric tables which has 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. Volume A2, covering classes 1–61 for the years 1966–69, is in preparation.

The work of the Crystallographic Data Centre is supported by the Office for Scientific and Technical Information, Department of Education and Science, and, since April 1974, by the Science Research Council 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. 1–5. 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 1974*

*Olga Kennard*
*David G. Watson*
*Frank H. Allen*
*Stella M. Weeds*

# Acknowledgements

The production of this bibliography was a collaborative effort by members of the Crystallographic Data Centre: Mrs A. Doubleday, Dr W. D. S. Motherwell, Miss S. A. Stephenson, Dr W. G. Town and Mrs K. A. M. Watson.

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

Mrs Doubleday has been responsible for scientific checking, registration of new entries and file editing.

Drs Town and Motherwell have written computer programs for the editing of the file.

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. G. Owston, Professor M. R. Truter and Professor A. J. C. Wilson, FRS (Chairman). We are indebted to Professor R. A. Raphael, FRS of the University Chemical Laboratory for his help and interest in our activities.

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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.

# Changes in Classification Rules

To regularise the classification procedures it was considered necessary to order the 86 chemical classes according to a precedence rule. Thus, for example, if a compound can be described as belonging to classes 15 and 17 then we will always assign 17 as the basic class with a cross-reference to 15, not vice-versa.

The order of precedence is indicated below running from top to bottom and left to right (i.e. class 61 has highest precedence and class 5 the lowest):

61, 60
71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 86, 85, 84, 83
70, 69, 68, 67, 66, 65, 64, 63, 62
58, 57, 56, 55, 54, 53, 52, 51, 50, 49, 48, 47, 46, 45, 44, 43, 59
42, 41, 40, 39, 38, 37, 36, 35, 34, 32, 33
31, 30, 29, 28, 27, 23, 22, 20, 21, 26, 25, 24
18, 14, 13, 17, 16, 15
2, 1, 3, 4
12, 8, 11, 7, 10, 9, 6, 19, 5

In addition to the above precedence rule the classification conventions have been better defined for classes 1–59. Some notes on specific classes are given below:

Class 1: Cyclic acid derivatives, e.g. anhydrides and lactones, are classified in the appropriate hetero-class. This rule applies also to class 13.

Class 2: In a few cases where the cation is organic we classify the anion in 2.

Class 4: The compound must contain –C–N–S– or –C–S–N–.

Class 9: The compound must contain –C–N–N–.

Class 10: The compound must contain –C–N–O– or –C–O–N–.

Class 24: The compound must be fully unsaturated.
The same rule applies to classes 25 and 26.

Class 44: The ring system must conform to the unmodified pyrimidine or purine skeleton.

Class 48: This class is reserved for peptides and $\alpha$-amino-acids, whether or not the amino-acid possesses biological properties. Thus a $\beta$-amino-acid would be classified in the appropriate acid and amine classes.

Class 50: A cross-reference to a structural class must be provided. This rule applies also to class 59.

# Contents

# List of Classes

# ALIPHATIC CARBOXYLIC ACID DERIVATIVES

1.C **Potassium hydrogen bis(dichloroacetate)**
$CH_2Cl_2O_2$, $CHCl_2O_2^-$, $K^+$
For complete entry see 2.1

1.C **Rubidium hydrogen bis(trichloroacetate)**
$C_2HCl_3O_2$, $C_2Cl_3O_2^-$, $Rb^+$
For complete entry see 2.4

1.C **Hydrazinium hydrogen oxalate**
$C_2HO_4^-$, $H_5N_2^+$
For complete entry see 2.6

1.C **Deuterated hydrazinium hydrogen oxalate**
$C_2DO_4^-$, $D_5N_2^+$
For complete entry see 2.7

1.C **Ammonium hydrogen bis - chloroacetate (ferroelectric form, at 80°K)**
$C_2H_3ClO_2$, $C_2H_2ClO_2^-$, $H_4N^+$
For complete entry see 2.8

1.C **5,5 - Diethylbarbituric acid - acetamide complex**
$C_2H_5NO$, $C_8H_{12}N_2O_3$
For complete entry see 60.6

1.C **Sodium hydrogen malonate**
$C_3H_3O_4^-$, $Na^+$
For complete entry see 2.9

1.C **Cyclohexylammonium phosphoenolpyruvate**
$C_3H_4O_6P^-$, $C_6H_{14}N^+$
For complete entry see 46.2

1.1 $\alpha$ - **Cyanoacetohydrazide**
$C_3H_5N_3O$
P.C.Chieh *J. C. S. Perkin II,* 1825, 1973
Also classified in 7, 9

1.C **1,7 - Diacetoxy - 2,4,6 - trinitro - 2,4,6 - triazaheptane - N,N - dimethylformamide complex**
$C_3H_7NO$, $C_8H_{14}N_6O_{10}$
For complete entry see 60.12

**1.C** **Sodium hydrogen acetylenedicarboxylate dihydrate**
$C_4HO_4^-$, $Na^+$, $2H_2O$
For complete entry see 2.10

**1.C** **Ammonium hydrogen acetylenedicarboxylate**
$C_4HO_4^-$, $H_4N^+$
For complete entry see 2.11

**1.2** **Acetylene dicarboxylic acid**
$C_4H_2O_4$
A.C.Larson, D.T.Cromer *Acta Cryst. (B)*, **29,** 1579, 1973

**1.3** **Maleic acid**
$C_4H_4O_4$
M.N.G.James, G.J.B.Williams *Acta Cryst. (B)*, **30,** 1249, 1974

**1.C** **Dipotassium tetrahydrogen trifumarate (neutron study)**
$C_4H_4O_4$, $2C_4H_3O_4^-$, $2K^+$
For complete entry see 2.14

**1.C** **Potassium hydrogen oxydiacetate**
$C_4H_5O_5^-$, $K^+$
For complete entry see 2.16

**1.C** **Potassium hydrogen oxydiacetate (neutron study)**
$C_4H_5O_5^-$, $K^+$
For complete entry see 2.17

**1.C** **Sodium hydrogen oxydiacetate**
$C_4H_5O_5^-$, $Na^+$
For complete entry see 2.18

**1.C** **Rubidium hydrogen oxydiacetate**
$C_4H_5O_5^-$, $Rb^+$
For complete entry see 2.19

**1.C** **Rubidium hydrogen oxydiacetate (neutron study)**
$C_4H_5O_5^-$, $Rb^+$
For complete entry see 2.20

**1.C** **Potassium trihydrogen disuccinate (neutron study)**
$C_4H_6O_4$, $C_4H_5O_4^-$, $K^+$
For complete entry see 2.15

**1.4** **Oxydiacetic acid (monoclinic form)**
Diglycollic acid
$C_4H_6O_5$
G.Davey, S.H.Whitlow *J. Cryst. Mol. Struct.*, **3,** 193, 1973

**1.5** **Oxydiacetic acid (monoclinic form)**
Diglycollic acid
$C_4H_6O_5$
H.Herbertsson, C.-E.Boman *Acta Chem. Scand.*, **27,** 2234, 1973

**1.6** $\gamma$ - **Aminobutyric acid (at −135°C)**
$C_4H_9NO_2$
E.G.Steward, R.B.Player, D.Warner *Acta Cryst. (B),* **29,** 2038, 1973
Also classified in 3

**1.7** $\gamma$ - **Aminobutyric acid**
$C_4H_9NO_2$
K.-I.Tomita, H.Higashi, T.Fujiwara *Bull. Chem. Soc. Jap.*, **46,** 2199, 1973
Also classified in 3

**1.8** $\beta$ - **Guanidinopropionic acid**
$C_4H_9N_3O_2$
E.G.Steward, D.Warner, G.R.Clarke *Acta Cryst. (B),* **30,** 813, 1974
Also classified in 8

**1.9** $\gamma$ - **Aminobutyric acid hydrochloride**
$C_4H_{10}NO_2^+$, $Cl^-$
E.G.Steward, R.B.Player, D.Warner *Acta Cryst. (B),* **29,** 2825, 1973
Residue 1 also classified in 3

**1.10** **Itaconic acid**
$C_5H_6O_4$
R.L.Harlow, C.E.Pfluger *Acta Cryst. (B),* **29,** 2965, 1973

**1.11** **DL - Methylsuccinic acid (monoclinic form)**
$C_5H_8O_4$
Y.Schouwstra *Acta Cryst. (B),* **29,** 1636, 1973

**1.12** **DL - Methylsuccinic acid (triclinic form)**
$C_5H_8O_4$
Y.Schouwstra *Acta Cryst. (B),* **29,** 1636, 1973

**1.C** **Potassium hydrogen trans - aconitate dihydrate**
$C_6H_5O_6^-$, $C_6H_4O_6^{2-}$, $3K^+$, $2H_2O$
For complete entry see 2.21

**1.13** **Dilactylamide**
$C_6H_{12}N_2O_3$
L.Mazzarella, C.Pedone, R.Puliti *Acta Cryst. (B),* **29,** 2699, 1973

**1.C** **Potassium hydrogen $\alpha$ - isopropyl - malate hydrate (absolute configuration)**
$C_7H_{11}O_5^-$, $K^+$, $xH_2O$
For complete entry see 2.22