Molecular Structures and Dimensions

Bibliography
1969-71
Organic and
Organometallic
Crystal
Structures

Edited by

Olga Kennard and David G Watson

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Vol. 3 Bibliography 1969-71 Organic and Organometallic Crystal Structures

Edited by Olga Kennard and David G. Watson 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

viii

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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).

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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.

Contents

1	Introduction	page vii
2	Acknowledgements	ix
3	List of Classes in Vol. 3	xi
4	Entries for Classes 1-86	1
5	Cumulative Formula Index for Vols. 1-3	F1
6	Cumulative Transition Metal Index for Vols. 1-3	M1
7	Cumulative Author Index for Vols. 1–3	Αl

List of Classes

1	Aliphatic Carboxylic Acid Derivatives	1
2	Aliphatic Carboxylic Acid Salts	
	(Ammonium, IA, IIA Metals)	6
3	Aliphatic Amines	9
4	Aliphatic (N and S) Compounds	*
5	Aliphatic Miscellaneous	17
6	Enolates (Aliphatic and Aromatic)	19
7	Nitriles (Aliphatic and Aromatic)	20
8	Urea Compounds (Aliphatic and Aromatic)	23
9	Nitrogen-Nitrogen Compounds (Aliphatic and Aromatic)	26
10	Nitrogen-Oxygen Compounds (Aliphatic and Aromatic)	30
11	Sulphur and Selenium Compounds	32
12	Carbonium Ions, Carbanions, Radicals	38
13	Benzoic Acid Derivatives	40
14	Benzoic Acid Salts	
	(Ammonium, IA, IIA Metals)	*
15	Benzene Nitro Compounds	44
16	Anilines	48
17	Phenols and Ethers	52
18	Benzoquinones	57
19	Benzene Miscellaneous	59
20	Monocyclic Hydrocarbons (3, 4, 5-Membered Rings)	62
21	Monocyclic Hydrocarbons (6-Membered Rings)	65
22	Monocyclic Hydrocarbons (7, 8-Membered Rings)	68
23	Monocyclic Hydrocarbons (9- and Higher-Membered Rings)	69
24	Naphthalene Compounds	71
25	Naphthoquinones	73
26	Anthracene Compounds	74
27	Hydrocarbons (2 Fused Rings)	76
28	Hydrocarbons (3 Fused Rings)	78

29	Hydrocarbons (4 Fused Rings)	80
30	Hydrocarbons (5 or More Fused Rings)	82
31	Bridged Ring Hydrocarbons	84
32	Hetero-Nitrogen (3, 4, 5-Membered Monocyclic)	89
33	Hetero-Nitrogen (6-Membered Monocyclic)	94
34	Hetero-Nitrogen (7- and Higher-Membered Monocyclic)	101
35	Hetero-Nitrogen (2 Fused Rings)	102
36	Hetero-Nitrogen (More than 2 Fused Rings)	105
37	Hetero-Nitrogen (Bridged Ring Systems)	111
38	Hetero-Oxygen	113
39	Hetero-Sulphur and Hetero-Selenium	120
40	Hetero-(Nitrogen and Oxygen)	126
41	Hetero-(Nitrogen and Sulphur)	129
42	Hetero-Mixed Miscellaneous	133
43	Barbiturates	134
44	Pyrimidines and Purines	136
45	Carbohydrates	145
46	Phosphates	154
47	Nucleosides and Nucleotides	157
48	Amino-Acids and Peptides	161
49	Porphyrins and Corrins	167
50	Antibiotics	169
51	Steroids	174
52	Monoterpenes	180
53	Sesquiterpenes	181
5 4	Diterpenes	185
55 56	Sesterterpenes	188
50 57	Triterpenes	189
5 <i>i</i>	Tetraterpenes Alkaloids	191
59	Miscellaneous Natural Products	192
60	Molecular Complexes	199 204
61	Clathrates	204
62	Boron Compounds	214
63	Silicon Compounds	210
64	Phosphorus Compounds	222
65	Arsenic Compounds	230
66	Antimony and Bismuth Compounds	230
67	Groups IA and IIA Compounds	232
68	Group III Compounds	237
69	Germanium, Tin, Lead Compounds	240
70	Tellurium Compounds	245
, ,		2-73

71	Transition Metal-C Compounds	246
72	Metal π-Complexes (Open-Chain)	256
73	Metal π-Complexes (Cyclopentadiene)	263
74	Metal π-Complexes (Arene)	272
75	Metal π-Complexes (Miscellaneous Ring Systems)	275
76	Metal Complexes (Ethylenediamine)	282
77	Metal Complexes (Acetylacetone)	292
78	Metal Complexes (Salicylic Derivatives)	298
79	Metal Complexes (Thiourea)	302
80	Metal Complexes (Thiocarbamate or Xanthate)	305
81	Metal Complexes (Carboxylic Acid)	308
82	Metal Complexes (Amino-Acid)	315
83	Metal Complexes (Nitrogen Ligand)	319
84	Metal Complexes (Oxygen Ligand)	343
85	Metal Complexes (Sulphur or Selenium Ligand)	351
86	Metal Complexes (Phosphine or Arsine Ligand)	360

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

- 1.C Formic acid formamide complex (at $-187 \,^{\circ}$ C) CH₂O₂, CH₃NO 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
- I.1 N Bromoacetamide

 C₂H₄BrNO

 R.J.Dubey Acta Cryst. (B), 27, 23, 1971
- 1.2 Acetic acid (at 5 ° C)

 C₂H₄O₂

 I.Nahringbauer Acta Chem. Scand., 24, 453, 1970
- 1.3 Acetic acid (at -190 ° C)

 C₂H₄O₂

 I.Nahringbauer Acta Chem. Scand., 24, 453, 1970
- 1.4 Acetic acid (neutron study, at −140 ° C) C₂H₄O₂ 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 C₂H₄O₃ W.P.Pijper Acta Cryst. (B), 27, 344, 1971
- Glycolic acid (neutron study)
 C₂H₄O₃
 R.D.Ellison, C.K.Johnson, H.A.Levy Acta Cryst. (B), 27, 333, 1971
- 1.7 Acetamide hemihydrobromide

 C₂H₆NO⁺, C₂H₅NO, Br⁻

 J.Weimann, H.Gillier-Pandraud, N.Thoai, C.Beaute

 Bull. Soc. Chim. Fr., 2147, 1969

1.8 Fluoromalonic acid

C₁H₁FO₄

G.Roelofsen, J.A.Kanters, J.Kroon, J.A.Vliegenthart Acta Cryst. (B), 27, 702, 1971

1.9 Dichloromalonamide

C₃H₄Cl₂N₂O₂

J.A.Lerbscher, K.V.Krishna Rao, J.Trotter J. Chem. Soc. (A), 1505, 1971

1.10 Cvanoacetamide

 $C_3H_4N_2O$

P.C.Chieh, J.Trotter J. Chem. Soc. (A), 184, 1970

Also classified in 7

1.11 Malonamide

C₃H₆N₂O₂

P.C.Chieh, E.Subramanian, J.Trotter J. Chem. Soc. (A), 179, 1970

1.12 N - Methyl - chloroacetamide

C₃H₇ClNO

Y.Koyama, T.Shimanouchi, Y.Iitaka Acta Cryvt. (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

C₄H₄Cl₂O₃

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

C4H5NO3

F.L.Hirshfeld Acta Cryst. (B), 27, 769, 1971

1.16 Trinitrobutyric acid

C₄H₅N₃O₈

C.M.Bock

Amer. Cryst. Assoc., Abstr. Papers (Winter Meeting), 41, 1970

Also classified in 10

1.17 (-) - 2 - Bromosuccinamic acid (absolute configuration)

C₄H₆BrNO₃

Y.Murakami, Y.Iitaka Chem. Pharm. Bull., Jap., 17, 2397, 1969

1.18 Methylmalonic acid

C₄H₆O₄

J.L.Derissen Acta Cryst. (B). 26, 901, 1970

1.19 (+) - Tartaric acid (absolute configuration)

C4H6O6

H.Hope, U.de la Camp Nature, 221, 54, 1969

1.C Betaine hydrochloride

C4H12NO2+, C1-

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

C6H10O4S

E.Martuscelli, L.Mazzarella, R.Palumbo, C.Pedone

Ric. Sci., 39, 573, 1969

Also classified in 11

1.21 Dilactylamide (optically active)

C6H12N2O2

E.Martuscelli, L.Mazzarella, R.Palumbo, C.Pedone

Ric. Sci., 39, 573, 1969

1.C Carbamoylcholine bromide

C6H15N2O2+, Br-

For complete entry see 3.24

1.22 racemic - 3 - Bromo - 4,4 - dihydroxypimelic acid dilactone C7H7BrO4

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

C8H8Cl2O4

H.M.Einspahr, J.Donohue

Amer. Cryst. Assoc., Abstr. Papers (Summer Meeting), 91, 1968

1.25 p - Chlorocinnamide

C₉H₈CINO

D.Rabinovich J. Chem. Soc. (A), 2361, 1969

1.C p - Coumaric acid

C₉H₈O₃

For complete entry see 17.5

1.C Hippuric acid

C₉H₉NO₃

For complete entry see 13.9

1.26 Azelamide (at $-140 \circ C$)

C9H18N2O2

M. Hospital Acta Cryst. (B), 27, 484, 1971

1.27 Azelamide (at 120 ° C)

C9H18N2O2

M. Hospital Acta Cryst. (B), 27, 484, 1971

1.28 Azelamide

C9H18N2O2

M. Hospital Acta Cryst. (B), 27, 484, 1971

1.29 p - Bromophenacyl dichloroacetate

C₁₀H₇BrCl₂O₃

J.C.Calabrese, A.T.McPhail, G.A.Sim J. Chem. Soc. (B), 285, 1970

1.30 p - Bromophenacyl difluoroacetate

C₁₀H₇BrF₂O₃

J.C.Calabrese, A.T.McPhail, G.A.Sim J. Chem. Soc. (B), 285, 1970

1.31 2,2,4,4 - Tetramethyladipic acid

C₁₀H₁₈O₄

E.Benedetti, C.Pedone, G.Allegra Macromolecules, 3, 16, 1970

1.32 β - Phenylglutaric acid

C11H12O4

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

C16H13NO3

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

C16H14O2S

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)

C18H34O8

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)

C19H38O2

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

C20H16O5

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

C25H46Br2O5

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

2CHO₂-, Sr²⁺, 2H₂O

K.Osaki Ann. Rep. Scient. Works Fac. Sci. Osaka, 6, 13, 1958

2.2 Potassium oxalate monohydrate (neutron study)

C₂O₄²⁻, 2K⁺, H₂O

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