

RODD'S CHEMISTRY OF CARBON COMPOUNDS

A modern comprehensive treatise

SECOND EDITION

Edited by
S. COFFEY

and
MARTIN F. ANSELL

VOLUME IV PART C
HETEROCYCLIC COMPOUNDS

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VOLUME IV PART C

HETEROCYCLIC COMPOUNDS

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Five-membered heterocyclic compounds with two hetero-atoms in the ring
from Groups V and/or VI of the Periodic Table



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PREFACE TO VOLUME IV C

The planning and editing of the second edition of Rodd's Chemistry of Carbon Compounds was undertaken by Dr. S. Coffey, who sadly did not see the completion of the project. This volume, the first of the second edition to be published since his death, includes a tribute to Dr. Coffey, written by Dr. Malcolm Bruce, which was inserted in the Supplement III BC. At the time of Dr. Coffey's death four volumes, IV C, D, I and J, remained to be commissioned and published. The contents of this volume, IV C, and its companion, IV D, follow the plan devised by Dr. Coffey and cover five-membered heterocyclic compounds containing two or more hetero-atoms. This volume contains compounds of this class with two hetero-atoms and Volume IV D covers compounds with three or more hetero-atoms.

I have been fortunate in that Dr. Malcolm Sainsbury and Dr. Raymond Theobald agreed to write this volume. They have achieved a very fine review of the newer material which has been carefully integrated with the older material of the first edition. The literature coverage is up to January 1981. Although the manuscript was received in 1982, for various technical and personal reasons publication has unfortunately been delayed.

I am grateful to the authors for their clear exposition of the subject matter and to Elsevier Science Publishers and the printers for the high technical excellence of the production.

I am sure that this volume will provide a valuable guide to all those seeking their way among the more complex five-membered heterocyclic systems.

June 1985

Martin F. Ansell

Dr. SAMUEL COFFEY

Samuel Coffey was born in Nottingham on 21st January 1900. He was educated at Mundella School, and then at University College, Nottingham. After graduating with First Class Honours in Chemistry he moved to University College, London, where he held an 1851 Exhibition Scholarship, and, in 1911, gained the degree of M.Sc. He continued academic research at the University of Leyden, and was awarded his D.Sc. in 1923 for work on cantharidin.

On arrival in Leyden he was informed by Professor Blanksma that discussions would be in English for two weeks, after which they would be in Dutch. He had some knowledge of German and French, and quickly learnt Dutch. His linguistic ability soon came to the notice of the editors of *Recueil des Travaux Chimiques des Pays-bas*, and he acted as a translator for them for the rest of his life.

Dr. Coffey returned to University College, London, as a Ramsay Memorial Fellow, and spent two years studying mercuration reactions. He was elected to Associateship of the Royal Institute of Chemistry in 1921, and to Fellowship four years later.

In 1925 he joined the Research Department of the British Dyestuffs Corporation, which in 1927 became the Dyestuffs Division of Imperial Chemical Industries Limited, sited at Blackley, Manchester. With the exception of four years in charge of research at the Huddersfield branch, he was based at Blackley until he retired, in 1962, having risen to the position of Personal Assistant to the Research Director.

His research at I.C.I. was mainly concerned with the chemistry of dyestuffs, and he headed groups working on indigoids, phthalocyanines and anthraquinones. Such was his expertise in the latter area that he was often referred to as 'Mr. Anthraquinone'. His friends called him Sam. He was author or co-author of some twenty papers and over sixty patents.

During the whole of his career at I.C.I., Dr. Coffey was involved in liaison between the Dyestuffs Division and the Universities, and he did much of this work in collaboration with Dr. E.H. Rodd, who was also at Dyestuffs Division, and who edited the ten volumes of the first edition of

'Chemistry of Carbon Compounds', published between 1951 and 1962 as a successor to Richter's 'The Chemistry of Carbon Compounds'.

As a tribute to Dr. Rodd's efforts, the second, current, edition was entitled 'Rodd's Chemistry of Carbon Compounds'. Sam Coffey agreed to edit it, starting in 1962, the year he retired from I.C.I. He never retired from Chemistry. That the publisher of 'Rodd', Elsevier, is based in Amsterdam was a happy coincidence, and served to strengthen the links with Holland which had begun in Leyden some forty years earlier.

Dr. Coffey was a meticulous Editor, always striving for perfection in the final manuscript, and for punctuality in its submission to the publisher. He was a constant source of encouragement and help to his authors, who were drawn from many branches of the scientific community, and was often to be found in the libraries of I.C.I. and the University of Manchester checking up on points of chemistry, biochemistry, and nomenclature. These visits led to happy reunions with his friends and former colleagues, and, of course, to discussions on chemistry. It is a tribute to his enthusiasm and industry that he edited twenty eight volumes of the second edition of 'Rodd'. He was working on the final volumes only three days before his death, on 5th March 1980.

The second edition of 'Rodd', under Dr. Coffey's guidance, has maintained, in a time of much more rapid expansion of knowledge, the standard of the first, and it still provides not only a valuable survey of current organic chemistry, but also an entry to the original literature for the researcher who requires information beyond the scope of the book. It is to be found worldwide in the libraries of Industry, the Universities, and Colleges, and, occasionally, in personal collections.

Dr. Coffey was Chairman of the Manchester Section of the Society of Chemical Industry from 1950 to 1961, and was the Society's representative on the Science Advisory Committee of Stockport College of Technology from early 1960 until the end of 1973. Such was his interest in education and in the College that he was then co-opted as a personal member, a position which he held until his death. His gift to the College Library of a copy of each of the volumes of 'Rodd' which he edited has been greatly appreciated.

He was keenly interested in the affairs of his local Parish Church for over forty years, and served on the Parochial Church Council Finance Committee, and as a Sidesman. He was a kind man, always willing to help those with whom he came in contact.

Sam Coffey was a dedicated family man. He is survived by his devoted wife, Ruth, to whom he was married in 1926, his sons John, a barrister, and

Robin, a chemist with I.C.I., and six grandchildren.

Sam Coffey was a scholar. His eighty years were full, productive, and happy. He will be widely remembered for his contributions to organic chemistry, to education, and to humanity. His friends will remember him with affection.

Manchester 1981

J. Malcolm Bruce

Titles of other parts of Volume IV

HETEROCYCLIC COMPOUNDS

- Vol. IV A:* Three-, four- and five-membered heterocyclic compounds with a single hetero-atom in the ring
- Vol. IV B:* Five-membered heterocyclic compounds with a single hetero-atom in the ring: alkaloids, dyes and pigments
- Vol. IV C:* Five-membered heterocyclic compounds with two hetero-atoms in the ring from Groups V and/or VI of the Periodic Table
- Vol. IV D:* Five-membered heterocyclic compounds with more than two hetero-atoms in the ring
- Vol. IV E:* Six-membered monoheterocyclic compounds containing oxygen, sulphur, selenium, tellurium, silicon, germanium, tin, lead or iodine as the hetero-atom
- Vol. IV F:* Six-membered heterocyclic compounds with a single nitrogen atom in the ring: pyridine, polymethylenepyridines, quinoline, isoquinoline and their derivatives
- Vol. IV G:* Six-membered heterocyclic compounds with a single nitrogen atom in the ring to which are fused two or more carbocyclic ring systems, and six-membered ring compounds where the hetero-atom is phosphorus, arsenic, antimony or bismuth. Alkaloids containing a six-membered heterocyclic ring system
- Vol. IV H:* Six-membered heterocyclic compounds with (a) a nitrogen atom common to two or more fused rings; (b) one hetero-atom in each of two fused rings. Six-membered ring compounds with two hetero-atoms from Groups VI B, or V B and VI B of the Periodic Table, respectively. Isoquinoline, lupinane and quinolizidine alkaloids
- Vol. IV I:* Six-membered heterocyclic compounds with two hetero-atoms from Group V of the Periodic Table: the Pyridazine and Pyrimidine groups
- Vol. IV J:* Six-membered heterocyclic compounds with two hetero-atoms from Group V of the Periodic Table: the Pyrazine group. Phenoxazine, phenothiazine, phenazine and sulphur dyes. Six-membered heterocyclic compounds with three or more hetero-atoms

- Vol. IV K:* Six-membered heterocyclic compounds with two or more hetero-atoms one or more of which are from Groups II, III, IV, V or VII of the Periodic Table. Heterocyclic compounds with seven or more atoms in the ring
- Vol. IV L:* Fused-ring heterocyclic compounds containing three or more nitrogen atoms; purines and related ring systems, nucleosides, nucleotides and nucleic acids; pteridines, alloxazines, flavins and related compounds. The biosynthesis of plant alkaloids and nitrogenous microbial metabolites

OFFICIAL PUBLICATIONS

B.P.	British (United Kingdom) Patent
F.P.	French Patent
G.P.	German Patent
Ger. Offen.	German Patent Application, open for inspection
Sw. P.	Swiss Patent
U.S.P.	United States Patent
U.S.S.R.P.	Russian Patent
B.I.O.S.	British Intelligence Objectives Sub-Committee Reports, H.M. Stationery Office, London.
C.I.O.S.	Combined Intelligence Objectives Sub-Committee Reports
F.I.A.T.	Field Information Agency, Technical Reports of U.S. Group Control Council for Germany
B.S.	British Standards Specification
A.S.T.M.	American Society for Testing and Materials
A.P.I.	American Petroleum Institute Projects
C.I.	Colour Index Number of Dyestuffs and Pigments

SCIENTIFIC JOURNALS AND PERIODICALS

With few obvious and self-explanatory modifications the abbreviations used in references to journals and periodicals comprising the extensive literature on organic chemistry, are those used in the World List of Scientific Periodicals.

LIST OF ABBREVIATED NAMES OF CHEMICAL FIRMS MENTIONED IN PATENT REFERENCES

A.G.F.A., Agfa A.G.	Aktiengesellschaft für Anilinfabrikation (Berlin)
B.A.S.F.	Badische Anilin- und Soda-Fabrik (Ludwigshafen)
Bayer	Farbenfabriken vorm. Friedrich Bayer und Co. (Leverkusen)
Cassella	Leopold Cassella und Co. (Frankfurt am Main)
C.F.M.	Compagnie française des Matières Colorantes (Paris)
CIBA	Gesellschaft für chemische Industrie (Basel)
Du Pont	E.I. Du Pont de Nemours and Co. (U.S.A.)
G.A.F.	General Anilin and Film Corporation (U.S.A.)
Geigy A.G.	J.R. Geigy S.A. (Basel)
Hoechst	Hoechst A.G. (see M.L.B.)
I.C.I.	Imperial Chemical Industries, Ltd. (London)
I.G.	(= Interessen Gemeinschaft Farbenindustrie) of the principal dyestuffs manufacturers in Germany
Kalle	Kalle und Co., A.G. (Biebrich am Rhein)
M.L.B.	Farbwerke vormals Meister, Lucius und Brüning (Hoechst)
Sandoz	Sandoz A.G. Chemische Fabrik (Basel)

LIST OF COMMON ABBREVIATIONS AND SYMBOLS USED

A	acid
Å	Ångström units
Ac	acetyl
<i>a</i>	axial
<i>as. asymm.</i>	asymmetrical
at.	atmosphere
B	base
Bu	butyl
b.p.	boiling point
C, mC and μ C	curie, millicurie and microcurie
<i>c, C</i>	concentration
c.d.	circular dichroism
conc.	concentrated
crit.	critical
D	Debye unit. 1×10^{-18} e.s.u.
<i>D</i>	dissociation energy
<i>D</i>	dextro-rotatory; dextro configuration
DL	optically inactive (externally compensated)
<i>d</i>	density
dec. or decomp.	with decomposition
deriv.	derivative
<i>E</i>	energy; extinction; electromeric effect
<i>E1, E2</i>	uni- and bi-molecular elimination mechanisms
ElcB	unimolecular elimination in conjugate base
e.s.r.	electron spin resonance
Et	ethyl
<i>e</i>	nuclear charge; equatorial
<i>f</i>	oscillator strength
f.p.	freezing point
<i>G</i>	free energy
g.l.c.	gas liquid chromatography
<i>g</i>	spectroscopic splitting factor, 2.0023
<i>H</i>	applied magnetic field; heat content
<i>h</i>	Planck's constant
Hz	hertz
<i>I</i>	spin quantum number; intensity; inductive effect
i.r.	infrared
<i>J</i>	coupling constant in n.m.r. spectra
<i>K</i>	dissociation constant
<i>k</i>	Boltzmann constant; velocity constant
kcal	kilocalories
<i>L</i>	laevorotatory; laevo configuration
<i>M</i>	molecular weight; molar; mesomeric effect
Me	methyl

<i>m</i>	mass; mole; molecule; <i>meta</i> -
ml	millilitre
m.p.	melting point
Ms	mesyl (methanesulphonyl)
[M]	molecular rotation
<i>N</i>	Avogadro number; normal
n.m.r.	nuclear magnetic resonance
N.O.E.	Nuclear Overhauser Effect
<i>n</i>	normal; refractive index; principal quantum number
<i>o</i>	<i>ortho</i> -
o.r.d.	optical rotatory dispersion
<i>P</i>	polarisation; probability; orbital state
Pr	propyl
Ph	phenyl
<i>p</i>	<i>para</i> -; orbital
p.m.r.	proton magnetic resonance
<i>R</i>	clockwise configuration
<i>S</i>	counterclockwise config.; entropy; net spin of incompleated electronic shells; orbital state
S_N1 , S_N2	uni- and bi-molecular nucleophilic substitution mechanisms
S_Ni	internal nucleophilic substitution mechanisms
<i>s</i>	symmetrical; orbital
<i>sec</i>	secondary
soln.	solution
symm.	symmetrical
<i>T</i>	absolute temperature
Tosyl	<i>p</i> -toluenesulphonyl
Trityl	triphenylmethyl
<i>t</i>	time
temp.	temperature (in degrees centigrade)
<i>tert</i>	tertiary
<i>U</i>	potential energy
u.v.	ultraviolet
<i>v</i>	velocity
α	optical rotation (in water unless otherwise stated)
$[\alpha]$	specific optical rotation
α_A	atomic susceptibility
α_E	electronic susceptibility
ϵ	dielectric constant; extinction coefficient
μ	microns (10^{-4} cm); dipole moment; magnetic moment
μ_B	Bohr magneton
μg	microgram (10^{-6} g)
λ	wavelength
ν	frequency; wave number

LIST OF COMMON ABBREVIATIONS

XXV

χ , χ_d , χ_μ	magnetic, diamagnetic and paramagnetic susceptibilities
\sim	about
(+)	dextrorotatory
(-)	laevorotatory
\ominus	negative charge
\oplus	positive charge

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VOLUME IV C

Heterocyclic Compounds: Five-membered heterocyclic compounds with two hetero-atoms in the ring from Groups V and/or VI of the Periodic Table

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