physical sciences data 35

organic colorants

a handbook of data of selected dyes for electro-optical applications

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21 A. Sala, **Radiant Properties of Materials. Tables of Radiant Values for Black Bodies and Real Materials**

Continued on page xvi

Preface

Dye chemistry, born in Europe at the end of the nineteenth century, is the root of modern organic chemistry, which in turn, together with inorganic and physical chemistry, has developed to produce polymer chemistry, biochemistry and the frontier materials science of today. Thus, dye chemistry is one of the foundations of our material civilization responsible for much of our everyday life. In spite of this fact, however, with the establishment of the dye industry and dye technology, the definition of dyes was narrowed and their study became estranged from the field of the general chemist. They were eventually abandoned as subjects of basic research. Recently, however, dyes have come to be reevaluated due to the progress made in frontier materials science. In Japan, at least, the concept of the functional dye has been established in information, display, recording and storage, energy conversion, medicine and other fields. The extraction, expansion, and utilization of the various functions of dyes have attracted much attention and a new field of color chemicals has come into being.

There are very few handy data books useful for chemists who wish to participate and contribute to the advance of molecular design or functional application of dyes. The best known work in this field, *Color Index*, is very large and cumbersome and geared mainly to professional dye chemists. The third and latest edition, published in 1971, is becoming somewhat outdated. Thus there is acute demand for the publication of an easy-to-use and functionally arranged data book on dyes which can be used by general chemists as well as by specialists.

This volume was compiled to meet this need and summarizes the absorption maximum, physical properties, end uses and the literature for 2,700 dyes which have been distinguished by their chromophores. The chemical structures of the major dyes are shown and the substituents for each dye are also described. We have put special effort into the indexes, which include a chemical name index, absorption maximum index and molecular formula index. We believe the publication

of this volume will provide easier access to the numerous possibilities inherent in color and materials chemistry.

The authors express their gratitude to Miss Kazuko Shirai for preparing the manuscript, and to the staff of Kodansha Scientific for its kind editorial assistance in producing the English version of this book.

April 22, 1988

The Authors

Organization of the Handbook

Following an introduction on the development and applications of special dyes, this volume is a compilation of data of some 2,700 selected dyes, including chemical structures, absorption spectra, properties and references. Indexes by chemical name, molecular formula, wavelength and end use of the dyes are found at the end of the volume.

Data for Organic Colorants

(1) All dyes are classified into the ten groups (I–X) shown below. Additional chromogens are shown in parentheses.

I.	Dye number 00000	Spiro compounds, Ferrocene, Fluorenone, Fulgide, Imidazole, Phenazine Phenothiazine
II.	Dye number 10000	Polyene (Carotene, Mareic anhydride, Pyrazolone, Stilbene, Styryl, Perylene)
III.	Dye number 20000	Azo compounds (Dithizone, Formazan)
IV.	Dye number 30000	Quinone (Phthaloylacridone, Anthanthrone, Indanthrone, Pyrenedione, Violanthrone)
V.	Dye number 40000	Indigo (Indirubin, Oxindigo, Thioindigo)
VI.	Dye number 50000	Diphenylmethane, Triphenylmethane (Fluoran, Fluorescein, Rhodamine)
VII.	Dye number 60000	Polymethine (Cyanine, Pyridinium, Pyrylium, Quinolinium, Rhodanine)

VIII.	Dye number 70000	Acridine, Acridinone, Carbostyril, Coumarin, Diphenylamine, Quinacridone, Quinophthalone, Phenoxazine, Phthaloperinone
IX.	Dye number 80000	Porphine, Chlorophyll, Phthalocyanine
X.	Dye number 90000	Others (Crown, Squarilium, Thiafulvalene)

The dye number is shown as a five-digit number. The first digit indicates group, the second chromophoric system and the third smaller group of chromophores. The fourth and fifth numbers show the derivatives of the dye.

Chemical name of the dye, chemical structure (subsitituent in brackets), molecular formula, and molecular weight are also given. Absorption maximum (λ_{max}) and molar absorptivity (log ε), fluorescent maximum (F_{max}), laser emission maximum (L_{max}) and sensitizing maximum (S_{max}) are shown.

Abbreviations for solvents are summarized as follows. The absorption maximum for each tautomeric isomer is also shown. Various properties, including melting point, p*K*a value, toxicity and others are listed. End use(s) is shown for each function, color index numbers are also shown, and references given.

Abbreviations for Solvents

A	ethanol
A/HCl	EtOH saturated with HCl
A/acid	EtOH-acid
A/base	EtOH-KOH(NaOH)
AA	acetic acid
Ac	acetone
AH	ammonium hydroxide
AN	acetonitrile
B	benzene
BA	butanol
BuAc	butyl acetate
BzA	benzyl alcohol
C	chloroform
CB	chlorobenzene
CD	carbon dioxide
CDS	carbon disulfide
CH	cyclohexane
CN	chloronaphthalene
CTC	tetrachloromethane
D	dioxane
DCB	dichlorobenzene
DCE	1, 2-dichloroethane
DCM	dichloromethane
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
E	ether
EA	ethyl acetate
EG	ethylene glycol
EGM	ethylene glycol monomethyl ether
FA	formic acid
H	*n*-hexane
HA	formamide
Hp	heptane
iOc	isooctane
iP	isopropyl alcohol
L	liquid state
LC	liquid crystal
M	methanol
MCH	methylcyclohexane
mCr	*m*-cresol
MEK	methyl ethyl ketone
MN	methylnaphthalene
NaLS	sodium lauryl sulfate
NB	nitrobenzene
NM	nitromethane
oCB	*o*-dichlorobenzene
oCP	*o*-chlorophenol
PB	petroleum benzine
PE	petroleum ether
PS	polystyrene
PVA	polyvinyl alcohol
Py	pyridine
S	solid state
T	toluene
TCA	trichloroacetic acid
TCB	trichlorobenzene
TCE	tetrachloroethane
TCET	tetrachloroethylene
TEA	triethylamine
TFA	trifluoroacetic acid
THF	tetrahydrofuran
V	vapor phase
W	water
X	xylene

Symbols for Property

λ_{max}	absorption maximum	S_{max}	sensitizing maximum
F_{max}	fluorescent maximum	D	dichroic ratio
L_{max}	laser emission maximum	S	sensitizing maximum

Abbreviations of the Literature

AB	Arch. Biochem.
ABB	Arch. Biochem. Biophys.
AC	Anal. Chem.
ACA	Anal. Chim. Acta
ACASH	Acta Chim. Acad. Sci. Hung.
ACP	Ann. Chim. (Paris)
ACR	Ann. Chim. (Rome)
ACS	Acta Chem. Scand.
AgC	Angew. Chem.
AJC	Australian J. Chem.
AK	Arkiv Kemi
Ann	Liebigs Annalen der Chemie
AP	Arch. Pharm.
APIP44	API Project 44, Spectra numbered 682-806, (1958-9)
BAPS	Bull. Acad. Polon, Sci.
BAPSS	Bull. Acad. Polon. Sci., Ser. Sci. Chim.
BAPSG	Bull. Acad. Polon. Sci., Ser. Sci. Chim., Geol., Geogr.
BBGPC	Ber. Bunsen-Gesellschaft. Phys. Chem.
BCSJ	Bull. Chem. Soc. Japan
Bio	Biochemistry
BJ	Biochem. J.
BSA	Boll. sedute accad. Gioenia sci. nau. Catania
BSCBe	Bull. soc. chim. Belges
BSCBi	Bull. soc. chim. biol.
BSCF	Bull. soc. chim. France
BSCF5	Bull. soc. chim. France, Series 5
BSFC	Boll. sci. fac. chim. ind. Bologna
CA	Chemical Abstracts
CB	Chemische Berichte
CC	Chemical Communications
CCCC	Coll. Czech. Chem. Comm.
CCOM	*Colour and Constitution of Organic Molecules*, J. Griffiths, Academic Press, London, 1976
CH	Chimia
CR	Chemical Reviews

CI	*Colour Index*, Third ed., eds. The Society of Dyers and Colourists, American Association of Textile Chemists and Colorists, London, 1971.
CIL	Chem. and Ind. (London)
CJC	Can. J. Chem.
CL	Chemistry Letters
CoR	Compt. rend.
CPBJ	Chem. Pharm. Bull. Japan
DAN	Dok. Akad. Nauk, S.S.S.R.
DOC	*Dictionary of Organic Compounds*, Fifth ed., ed. J. Buckingham, Chapman and Hall, New York, 1982
DP	Dyes and Pigments
DPh	Die Pharmazie
Eastman	Kodak Laser Products, Kodak Publication No. JJ-169, 1982
EJC	Egyptian J. Chem.
EJCSI	Egyptian J. Chem., Special Issue
FWA	Fluorescent Whitening Agents, R. Anliker, G. Müller, Georg Thieme Publishers, Stuttgart, 1975
GCI	Gazz. chim. ital.
HCA	Helv. Chim. Acta
HUVOC	*Handbook of Ultraviolet and Visible Absorption Spectra of Organic Compounds*, K. Hirayama, Plenum Press, New York, 1967
IAN	Izv. Akad. Nauk S.S.S.R.
IECA	Ind. Eng. Chem., Anal. Ed
IJC	Indian J. Chem.
JACB	J. Appl. Chem. Biotech.
JACS	J. Am. Chem. Soc.
JAnC	J. Anal. Chem. U.S.S.R.
JAPAS	J. Am. Pharm Assoc.. Sci. Ed.
JApC	J. Appl. Chem. U.S.S.R.
JBC	J. Biol. Chem.
JCED	J. Chem. Eng. Data
JCiP	J. chim. phys.
JCP	J. Chem. Phys.
JCS	J. Chem. Soc.
JCSF1	J. Chem. Soc., Faraday Trans.I
JCSP1	J. Chem. Soc., Perkin Trans.I
JCSP2	J. Chem. Soc., Perkin Trans. II
JCSSB	J. Chem. Soc., Sect. B
JCSSC	J. Chem. Soc., Sect. C
JHC	J. Heterocyclic Chem.
JICS	J. Indian Chem. Soc.
JINC	J. Inorg. Nucl. Chem.
JMC	J. Med. Chem.
JMoSp	J. Mol. Spectroscopy
JMoSt	J. Mol. Structure

JOC	J. Org. Chem.
JOSA	J. Optical Soc. Am.
JPhC	J. Phys. Chem.
JPhSJ	J. Pharm. Soc. Japan
JPoSA	J. Polymer Sci., Pt. A-1
JPrC	J. prakt. Chem.
JSDC	J. Soc. Dyers and Colourists
JSOC	Yuki Gosei Kagaku Kyokaishi (J. Soc. Org. Syn. Chem., Tokyo)
KGS	Khim. Geterosikl. Soedin.
KK	Kogyo Kagaku Zasshi (J. Soc. Japan, Industrial Chemistry Section)
LAOC	*Light Absorption of Organic Colorants*, J. Fabian, H. Hartmann, Springer-Verlag, Berlin, 1980
LC	Proceedings of 9th Liquid Crystal Symposium, Chem. Soc. Japan, 1983
MA	Mikrochimica Acta
Moc	Monatsh. Chem.
MUCB	Moscow Univ. Chem. Bull.
NDVS	Nauch. Doklady Vysshei Shkoly, Khim. i. Khim. Technol.
NK	Nippon Kagaku Kaishi (J. Chem. Soc. Japan, Chemisty and Industrial Chemistry, Japan)
NKS	Catalogs of Nippon Kankoh Shikiso Kenkyusho Co., Ltd., 1972
NKZ	Nippon Kagaku Zasshi (J. Chem. Soc. Japan, Pure Chemistry Section)
OES	*Organic Electronic Spectra Data*, eds., J. P. Phillips *et al.*, John Wiley & Sons, New York, (1956~)
OSM	*Optical Storage Media SPIE-420, eds.* A. E. Bell, A. A. Jamberdino, Washington, 1983
PH	*Pigment Handbook*, ed. T. C. Patlon, John Wiley & Sons, London, 1973
Photo	Photochromism, ed. G. H. Brown, Techniques of Chemistry, Vol. 3, Wiley Interscience, 1971
Phy	Phytochemistry
PIAS	Porc. Iowa Acad. Sci.
PMP	*Porphyrins and Metalloporphyrins*, ed. Kevin M. Smith, Elsevier Scientific Publishing Company, 1975
RC	Roczniki Chem.
RJPC	Russian J. Phys. Chem.
RPC	*Review of Progress in Coloration*, The Society of Dyers and Colourists, Bradford, (1970–1985)
RRC	Revue Roumaine Chim.
RTC	Rec. trav. chim.
SA	Spectrochim. Acta
SK	Shikizai Kyokai Shi (J. Japan Soc. Colour Material)
Sy	Synthesis

Tal	Talanta
Tet	Tetrahedron
TFS	Trans. Faraday Soc.
TL	Tetrahedron Letters
UKZ	Ukrain. Khim. Zhur.
ZC	Z. Chemie
ZE	Z. Electrochem.
ZN	Z. Naturforsch.
ZObK	Zhur. Obshchei Khim.
ZOrK	Zhur. Organ. Khim.
ZPCF	Z. phys. Chem. (Frankfurt)
ZPCL	Z. phys. Chem. (Leipzig)

Continued from page ii

22 O.Söhnel and P.Novotny, **Densities of Aqueous Solutions of Inorganic Substances**
23 J.Wisniak and A.Tamir, **Liquid-Liquid Equilibrium and Extraction, Supplement 1**
24 R.Poirier, R.Kari and I.G.Csizmadia, **Handbook of Gaussian Basis Sets**
25 B.D.Smith and R.Srivastava, **Thermodynamic Data for Pure Compounds**
Part A. Hydrocarbons and Ketones
Part B. Halogenated Hydrocarbons and Alcohols
26 J.Wisniak and A.Tamir, **Mixing and Excess Thermodynamic Properties, Supplement 2**
27 J.Wisniak, **Phase Diagrams, Supplement 1**
28 J.Wisniak and A.Tamir, **Liquid-Liquid Equilibrium and Extraction. A Literature Source Book, Supplement 2**
29 R.A.Hites and W.J.Simonsick, Jr., **Calculated Molecular Properties of Polycyclic Aromatic Hydrocarbons**
30 J.R.Dias, **Handbook of Polycyclic Hydrocarbons**
Part A. Benzenoid Hydrocarbons
Part B. Polycyclic Isomers and Heteroatom Analogs of Benzenoid Hydrocarbons
31 G.Hradetzky, I.Hammerl, H.-J.Bittrich, K.Wehner and W.Kisan, **Selective Solvents. Data on Dimethylformamide-N-methylcaprolaction-N-methylpyrrolidone**
32 J.L.Delcroix, **Gas-Phase Chemical Physics Database**
33 Y.C.Jean, R.M.Lambracht and D.Horvath, **Positrons and Positronium. A Bibliography 1930-1984**
34 T.Shida, **Electronic Absorption Spectra of Radical Ions**
35 M.Okawara, T.Kitao T.Hirashima and M.Matsuoka, **Organic Colorants. A Handbook of Data of Selected Dyes for Electro-optical Applications**

Contents