CODE USED FOR DESCRIBING ANALYTICAL METHODS

Analytical procedures have been abstracted, using the following symbols:

1. Capital letters refer to either the type of sample used or the unit operations of the procedure.
2. Lower case letters refer to the solvent or reagent used in that operation.

SAMPLE

B...Blood R...Air T...Tissue U...Urine Z...General Sample

UNIT OPERATION

A....Absorption

AA..Atomic Absorption

C....Chromatography
- *Cc*..column
- *Cg*..gas
- *Cp*..paper
- *Ct*..thin-layer

D....Dissolve

E....Extraction

F....Fluorometry (subscript for excitation and emission, *e.g.*, $F_{380/440}$)

G....Filtrate

H....Hydrolysis

J.... Reflux

K....Ashing

L....Colorimetric Reaction

M...Titration

N... Distillation

P....Precipitation

Protein Precipitation
- *Pi*...trichloracetic acid
- *Ps*...ammonium sulfate
- *Pw*.. tungstate
- *Pz*...zinc and alkali

Phos. Phosphorimetry

S....Spectrophotometry (wavelength as a subscript, *e.g.*, S_{256})
- *Suv*..Ultraviolet Spectrophotometry
- *Sir* ..Infrared Spectrophotometry

V....Evaporate

W...Separation

Y... Saponification

SOLVENTS

a..acid

b..base

c..chloroform

d..ethylene dichloride

e..ether

f..ethanol

h..heptane

j..water

k..ethyl acetate

l...petroleum ether

m..methanol

n...methylene dichloride

o...other (specified)

r...benzene

t...dimethylformamide

u...acetone

v...acetonitrile

x...hexane

y...higher aliphatic alcohols

Illustration: B, P*i*, N*b*, E*bc*, E*a*, E*be*, V, W*u*, C*g*

The proteins in the sample of blood are precipitated by trichloracetic acid. The filtrate is made alkaline and distilled. The distillate is made basic and extracted with chloroform. The chloroform is extracted with acid and this in turn is made basic and extracted with ether. The ether is evaporated and the residue is dissolved in acetone. The acetone is used for gas chromatographic analysis.

"L" has been used to indicate that a series of special reagents was added to the system to produce a chemical change required in the analysis.

PREFACE

This handbook collates, in one volume, many data that are essential to scientists concerned with the analysis of drugs, environmental hazards, economic poisons and industrial chemicals. Subsequent volumes will supply those data unavailable for this first edition. This improvement will ensue as more scientists, in their interest to have a more valuable desk-side handbook, recognize the value of this compendium and willingly volunteer to fill the gaps.

In addition to collating the physical and chemical properties of drugs and chemical hazards, summaries of published methods for their detection in biological specimens are presented. The minutiae of the analyses are beyond this volume, but the reader is given an insight into the analytical approach to the analysis of many compounds and a specific reference wherein the essential details can be found. These references will help those analysts who are requested to determine one of the many substances listed in the handbook with which they have had no previous analytical experience. Frequently, the converse is true. The analyst elaborates a series of physical and chemical facts about an "unknown substance" and has to try to determine its identity. To facilitate this, the various chemical and physical properties of each substance have been arranged in sequential order in a separate section of the handbook. These compilations should help the analyst narrow the list of probabilities and identify the "unknown substance". Their potential value will increase as the data grow in volume.

The result of a quantitative analysis is usually interpreted by comparing it with suitable reference data. These data, as they refer to exposed humans, have been collected and tabulated. They should prove valuable, not only to analysts, but also to those who must interpret analytical results—physicians, pharmacologists, toxicologists, industrial hygienists and scientists in the drug industry and governmental agencies. Since many of these scientists are also interested in how the body handles the products described, data on human absorption, excretion and metabolism also have been assembled and tabulated for easy reference.

The facts presented in this volume originate from many different sources. Editorial selection has been made to present the best available data. Since many were obtained in different laboratories, using different instruments or reference substances of varying degrees of purity, the reported values may differ from those of primary standards for the same substances, where available. Since the latter are seldom available and usually are not those involved in daily problems, the published data should be adequate.

Many contributors provided the data for this volume. Without their help, the handbook would not have been possible. Everyone is indebted to them for their assistance. May this continue and be augmented by others so that subsequent volumes will be even more valuable.

Irving Sunshine

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Compilations and contributions notwithstanding this volume would never have been completed were it not for the diligent, continuous, encompassing efforts of Barbara Cramer, the Administrative Editor. Her painstaking care with all the minutiae of manuscript and galley preparation kept errors to a minimum and format uniform and crisp. Much of whatever credit there is for this volume must be hers.

INTRODUCTION

This Handbook has three major sections. Each section is further divided into units on drugs, economic poisons, industrial chemicals, air and water pollutants. Material in the first section is arranged alphabetically so that information about a specific substance can be easily located.

Each unit in the first section contains an alphabetically arranged index which includes common synonyms, cross-referenced to the accepted names. This is followed by a tabulation of the accepted names, chemical names, the Chemical Abstracts Registry Number, when known, and structural formulas. A third tabulation includes the physical properties, toxicity data and a brief description of published analytical methods for the detection of a given substance in biological samples. Depending on their availability, tables containing additional physical, toxicological or analytical data are presented in some units.

The second section is a sequential tabulation of physical properties. These tables are designed to facilitate the identification of unknown substances whose physical properties have been elaborated during the course of an analysis. Many substances may have similar values for a given physical property, such as a melting point, an R_f value in a given solvent or an ultraviolet absorption maximum. The analyst can use the sequentially arranged tables to determine which substances are compatible with a given physical constant. Repeating this comparison for the several constants revealed in a given analysis will yield several groups. The unknown can be identified by noting the one substance that appears in each of these groups.

The third section presents a brief discussion of some physical methods of instrumental analysis and their application to substances of toxicological interest. Bibliographic appendices are included for those who have the equipment described in Section III and want to apply it to the analysis of particular substances.

Section four consists of a detailed index. The various items contained in each unit have been tabulated opposite the name of each product so that the reader may more easily find the specific information he seeks. For easy access, the index has been sub-divided into units on drugs, economic poisons and industrial chemicals. These units are followed by a general index encompassing all other material.

Usage Common to all Tabulations

Optimal nomenclature is a relatively subjective choice. Many acceptable systems are in common use. Arbitrarily, the names accepted for use in this Handbook and their chemical formulas conform as closely as possible with the system of nomenclature adopted by the International Union of Pure and Applied Chemistry and used by the Chemical Abstracts Service, American Chemical Society. Some of the sources for the other recorded data include the "Handbook of Chemistry and Physics," 49th edition, Robert C. Weast, Ed., The Chemical Rubber Co., Cleveland, Ohio, 1968; "The Merck Index," 8th edition, Paul G. Stecher, Ed., Merck & Co., Inc., Rahway, N.J., 1968; "The Extra Pharmacopoeia, Martindale," 25th edition, R. G. Todd, Ed., The Pharmaceutical Press, London, 1967; "The Pharmacopoeia of the U.S.A.," 17th edition, Mack Printing Co., Easton, Pa., 1965; "Analytical Methods for Pesticides, Plant Growth Regulators and Food Additives," Vol. I, II, III, IV, V, Gunter Zweig, Ed., Academic Press, New York, N.Y., 1963-1967; "Guide to The Analysis of Pesticide Residues," Vol. I, II, H. P. Burchfield and Donald E. Johnson, U.S. Department of Health, Education & Welfare, U.S. Public Health Service, Washington, D.C., 1965 and "Industrial Hygiene and Toxicology," Vol. II, Frank A. Patty, Ed., Interscience Publishers, Inc., New York, N.Y., 1963; and "Pesticide Index," 3rd edition, Donald E. H. Frear, Ed., College Science Publishers, State College, Pa.

The Chemical Abstracts Registry Number was taken from the 1965 SOCMA Handbook of Commercial Organic Chemical Names or was provided by the Chemical Abstracts Service. This Registry Number uniquely identifies organic compounds and serves to identify the compound throughout the CAS Registry System. Access to Chemical Abstracts and other computer-stored data using this number, may be obtained.

Solubility was expressed in the usual USP format which is the following:

USP descriptive solubility term	Symbol	Parts of solvent one part solute	Mg of solute/ 100 ml solvent	G of solute/ 100 ml solvent
Very	vs	less than 1	over 100,000	100
Freely	fs	from 1 to 10	100,000–10,000	100–10
Soluble	s	10 to 30	10,000–3,333	10–3.3
Sparingly	ss	30 to 100	3,333–1,000	3.3–1.0
Slightly	sls	100 to 1,000	1,000–100	1.0–0.1
Very slightly	vsl	1,000 to 10,000	100–10	0.1–0.01
Insoluble	in	more than 10,000		
Miscible	mis			

The Sadtler Reference Number refers to the compound's identification number in their collection of infrared absorption data. Space precludes publication of the actual absorption spectra, but the wavelength of the major absorption peak in each millimicron region is given in the Spec-Finder® data published in Section II.

The chromatographic data include an R_f value followed by a number in parentheses. This number refers to the Table in Section II which contains complete information on all the analytical parameters used to obtain the chromatographic data and original source of the data. Not only do these tables contain the available information for the given substance but they also include additional data on many related compounds, arranged in sequential order. If several spots were reported, the R_f of the major spot is listed. Whenever relative R_f data are presented, these data are italicized.

The general principles of the analytical procedures for the detection of the many substances listed in the Handbook are given in terms of the unit operations required to isolate and quantitate each substance. These unit operations were coded using capital letters to signify the several operations involved. Those common solvents required to carry out the extraction operations were designated by lower case italic letters. These codes were then used to describe each analytical procedure. Should the reader require specific details, the original source is cited using a number in the reference column. This number refers to the literature citation of the reference in question and will be found in the bibliography at the end of the Table. For ready access, the codes for the analytical procedures have been imprinted on both the inside back and front covers. With a little practice, decoding the procedures becomes relatively easy. As a guide, the following procedure is decoded:

B, P*i*, N*b*, E*bc*, E*a*, E*be*, V, W*u*, C*g*

The proteins in the sample of blood are precipitated by trichloracetic acid. The filtrate is made alkaline and distilled. The distillate is made basic and extracted with chloroform. The chloroform is extracted with acid and this in turn is made basic and extracted with ether. The ether is evaporated and the residue is dissolved in acetone. The acetone is used for gas chromatographic analysis.

The sources of the LD_{50} data were legion and cannot be referenced conveniently. The following explains the symbols used in this portion of the Table:

R—rat	s.c.—subcutaneous
M—mouse	i.m.—intramuscular
B—rabbit	i.v.—intravenous
D—dog	i.p.—intraperitoneal
GP—guinea pig	

In addition to the terminology and symbolism described above, other tabulations containing additional or other symbols will have suitable explanations as prefaces or footnotes.

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DRUGS

Many chemical agents are used for pharmaceutical purposes. Not all of these are of primary interest to toxicologists. Those substances which are included in this unit were selected because they represent the bulk of those active agents with which toxicologists may be concerned. Hormones, steroids, vitamins, antihelminthics, antineoplastic chemotherapeutic agents, important as they are, were not included in this edition. Also omitted were the many drug intermediates, various excipients and all inorganic agents.

Those physical properties that are most frequently used were tabulated in Table 1. The chromatographic data in that Table are put in better perspective in Section II, Unit I. In that Unit, they are tabulated in sequential order along with all other substances chromatographed in the same system. U.V. Absorption data could not be included in Table 1, so they appear in a separate compilation, Table 5. The actual spectra follow Table 5 and should prove to be a valuable resource.

Infrared spectra are not depicted. Key numbers, referred to in Table 1 as Sadtler Reference numbers, refer the reader to Spec-Finder® data in Section II. In this compilation, the major infrared absorption peak of the compound in question is listed as a function of each micron of its absorption curve.

Fluorometric properties will be found in Table 34, of Section III. Identification of microgram quantities of drugs by microscopy is sensitive, specific and elegant. The material in Tables 11 and 13 gives the results one can expect from microcrystalline tests and thermal microscopy.

Some or all of these data are used for the analytical tests described in Table 1. These tests, when applied to humans, yield data which are tabulated in Table 7. Herein, one will find reported blood and urine concentrations of a drug following a given dose. In addition, where the metabolites have been identified in human systems, they have been listed in this same Table.

More recent analytical techniques of mass spectrography, nuclear magnetic resonance, and X-ray diffraction have been applied to drugs, but these data are even more incomplete than those listed in Table 1, and were omitted from this volume. As they are compiled, they will be collated and serve as the nucleus for new material for Volume II of this Handbook.

TABLE 1. DRUGS—PHYSICAL, TOXICOLOGICAL

No.	Compound Molecular Formula Molecular Weight	C.A. Reg. No. (Sadtler IR Ref. No.)	M.P. °C	B.P. °C (mm/Hg)	pK_a	Solubility						
						H_2O	EtOH	$CHCl_3$	Et_2O	C_6H_6	Me_2CO	Other Solvents
1	**Acenocoumarol** $C_{19}H_{15}NO_6$ 353.3	152727 (R820)	196–199			ss						vsl., most organic solvents
2	**Acepromazine** $C_{19}H_{22}N_2OS$ 326.5	61007	(liq.)	220–240 (0.5)								
3	**Acepromazine maleate** $C_{19}H_{22}N_2OS \cdot C_4H_4O_4$ 442.5	3598376	135–136			s	ss	fs	sls			s, EtOAc
4	**Acetanilide** C_8H_9NO 135.2	103844	113–115	307 (760)	1	sls	fs	fs	s	ss	fs	fs, MeOH vs, pet. ether
5	**Acetazolamide** $C_4H_6N_4O_3S_2$ 222.3	59665 (R2)	258–259		7.2	ss	sls	in	in		ss	in, CCl_4
6	**Acetazolamide sodium** $C_4H_5N_4NaO_3S_2$ 244.2	1424277 (R3)				s						
7	**Acetohexamide** $C_{15}H_{20}N_2O_4S$ 324.4	968810	184–189		6.6	in	ss	in	in		ss	ss, dioxane
8	**Acetophenetidine** $C_{10}H_{13}NO_2$ 179.2	62442 (R6)	134–135			cold-vsl boil-ing-ss	s	s	ss			
9	**Acetylcarbromal** $C_9H_{15}BrN_2O_3$ 279.1	77667	109			sls	s	s	s			fs, EtOAc
10	**Acetylsalicylic acid** $C_9H_8O_4$ 180.2	50782 (R11)	135			sls	fs	s	s			
11	**Acetyl sulfisoxazole** $C_{13}H_{15}N_3O_4S$ 309.4	80740	192–195			in	sls	ss				
12	**Aconitine** $C_{34}H_{47}NO_{11}$ 645.7	1353704	204		8.35	vsl	s	fs	ss	fs		sls, pet. ether
13	**Aconitine HCl** $C_{34}H_{47}NO_{11} \cdot HCl$ 682.2	1378514	180 dec.			s	s					

AND ANALYTICAL DATA (Continued)

No.	Stability		Chromatography (Ref.)*			Analytical Methods *See* code on inside covers	Ref.	LD_{50} mg/kg	
	Air	Solution	Paper Rf	Thin-Layer Rf-*RRf*	Gas-Liquid Rt-*RRt*			Oral	Parenteral
1				0.20 (10)				R-513	
2			0.50 (1)	0.50 (23a) 0.45 (23b) 0.42 (44)				R-130	R-70 (i.v.)
3	Sensitive to light		0.92 (22)						
4						(B-T), E*ayd*, V, H*a*, L, S_{550} U, E*ayd*, V, H*a*, E*bry*, E*a*, L, S_{550}	104 104	R-800	
5	Sensitive to light			0.45 (11)					
6									
7				0.52 (33)		B, E*c*, *Cc*, V, D*f*, S_{228} B, E*ac*, E*b*, C*t*, $S_{247/228}$ U, E*ac*, V, *Cp*	170 105 235		
8			0.35 (21)	*0.26* (22a) *0.62* (22b) 0.67 (25c) 0.98 (55)	*2.25* (9) 5.7 (13a) *0.46* (21) *0.39* (45)	Z, E*yr*, V, E*a*, L, S_{300} T, E*ac*, V, D*a*, G, Ec, *Cp*, S_{272}	106 5	R-1700	
9	Sensitive to light	Dec. in boiling water			*See* ref. 12				
10		Dec. in boiling water and alkali		*0.20* (22a) *0.22* (22b) *0.30* (22c) 0.65 (59)	*0.34* (21) *0.09* (45)	B, P*w*, G*b*, $F_{310/410}$ Z, E*ad*, $E_{ferric\ nitrate}$, S_{525} B, P, S_{525} U, E*d*, E*a*, L, S_{525}	326 238 237 159	R-1750 M-1100 B-1800	R-500 (i.p.)
11				0.90 (62)					
12	Sensitive to light		0.65 (1) 0.94 (3a) 0.97 (3b)	0.35 (1a) 0.36 (1b) 0.60 (1c) 0.68 (37)	10.6 (18)			M-20	M-6.9 (i.v.)
13									

* Chromatographic references ( ) are located in Section II of this Handbook.