

Ullmann's Encyclopedia of Industrial Chemistry

Sixth, Completely Revised Edition

Volume 19

Laboratory Information
and Management
Systems (LIMS)
to
Liquid-Liquid
Extraction

 WILEY-VCH

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Ullmann's Encyclopedia of Industrial Chemistry

Volume 19

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Volume 40: Index

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Symbols and Units

Symbols and units agree with SI standards (for conversion factors see page IX). The following list gives the most important symbols used in the encyclopedia. Articles with many specific units and symbols have a similar list as front matter.

Symbol	Unit	Physical Quantity
a_B		activity of substance B
A_r		relative atomic mass (atomic weight)
A	m^2	area
c_B	mol/m^3 , mol/L (M)	concentration of substance B
C	C/V	electric capacity
c_p, c_v	$J\text{ kg}^{-1}\text{ K}^{-1}$	specific heat capacity
d	cm, m	diameter
d		relative density (ρ/ρ_{water})
D	m^2/s	diffusion coefficient
D	Gy (= J/kg)	absorbed dose
e	C	elementary charge
E	J	energy
E	V/m	electric field strength
E	V	electromotive force
E_A	J	activation energy
f		activity coefficient
F	C/mol	Faraday constant
F	N	force
g	m/s^2	acceleration due to gravity
G	J	Gibbs free energy
h	m	height
$\hbar$	$\text{W} \cdot s^2$	Planck constant
H	J	enthalpy
I	A	electric current
I	cd	luminous intensity
k	(variable)	rate constant of a chemical reaction
k	J/K	Boltzmann constant
K	(variable)	equilibrium constant
l	m	length
m	g, kg, t	mass
M_r		relative molecular mass (molecular weight)
n_D^{20}		refractive index (sodium D-line, 20 °C)
n	mol	amount of substance
N_A	mol^{-1}	Avogadro constant ($6.023 \times 10^{23} \text{ mol}^{-1}$)
p	Pa, bar *	pressure
Q	J	quantity of heat
r	m	radius
R	$J\text{ K}^{-1}\text{ mol}^{-1}$	gas constant
R	Ω	electric resistance
S	J/K	entropy
t	s, min, h, d, month, a	time

Symbols and Units (Continued from p. VII)

Symbol	Unit	Physical Quantity
t	$^{\circ}\text{C}$	temperature
T	K	absolute temperature
u	m/s	velocity
U	V	electric potential
U	J	internal energy
V	m^3 , L, mL, μL	volume
w		mass fraction
W	J	work
x_{B}		mole fraction of substance B
Z		proton number, atomic number
α		cubic expansion coefficient
α	$\text{W m}^{-2}\text{K}^{-1}$	heat-transfer coefficient (heat-transfer number)
α		degree of dissociation of electrolyte
$[\alpha]$	$10^{-2}\text{deg cm}^2\text{g}^{-1}$	specific rotation
η	$\text{Pa} \cdot \text{s}$	dynamic viscosity
θ	$^{\circ}\text{C}$	temperature
$\varkappa$		c_p/c_v
λ	$\text{W m}^{-1}\text{K}^{-1}$	thermal conductivity
λ	nm, m	wavelength
μ		chemical potential
ν	$\text{Hz} \cdot \text{s}^{-1}$	frequency
ν	m^2/s	kinematic viscosity (η/ρ)
π	Pa	osmotic pressure
ρ	g/cm^3	density
σ	N/m	surface tension
τ	$\text{Pa (N/m}^2\text{)}$	shear stress
φ		volume fraction
χ	$\text{Pa}^{-1} (\text{m}^2/\text{N})$	compressibility

* The official unit of pressure is the pascal (Pa).

Conversion Factors

SI unit	Non-SI unit	From SI to non-SI multiply by
<i>Mass</i>		
kg	pound (avoirdupois)	2.205
kg	ton (long)	9.842×10^{-4}
kg	ton (short)	1.102×10^{-3}
<i>Volume</i>		
m ³	cubic inch	6.102×10^4
m ³	cubic foot	35.315
m ³	gallon (U.S., liquid)	2.642×10^2
m ³	gallon (Imperial)	2.200×10^2
<i>Temperature</i>		
°C	°F	$^{\circ}\text{C} \times 1.8 + 32$
<i>Force</i>		
N	dyne	1.0×10^5
<i>Energy, Work</i>		
J	Btu (int.)	9.480×10^{-4}
J	cal (int.)	2.389×10^{-1}
J	eV	6.242×10^{18}
J	erg	1.0×10^7
J	kW · h	2.778×10^{-7}
J	kp · m	1.020×10^{-1}
<i>Pressure</i>		
MPa	at	10.20
MPa	atm	9.869
MPa	bar	10
kPa	mbar	10
kPa	mm Hg	7.502
kPa	psi	0.145
kPa	torr	7.502

Powers of Ten

E (exa)	10 ¹⁸	d (deci)	10 ⁻¹
P (peta)	10 ¹⁵	c (centi)	10 ⁻²
T (tera)	10 ¹²	m (milli)	10 ⁻³
G (giga)	10 ⁹	μ (micro)	10 ⁻⁶
M (mega)	10 ⁶	n (nano)	10 ⁻⁹
k (kilo)	10 ³	p (pico)	10 ⁻¹²
h (hecto)	10 ²	f (femto)	10 ⁻¹⁵
da (deca)	10	a (atto)	10 ⁻¹⁸

Abbreviations

The following is a list of the abbreviations used in the text. Common terms, the names of publications and institutions, and legal agreements are included along with their full identities. Other abbreviations will be defined wherever they first occur in an article. For further abbreviations, see page VII, Symbols and Units; page XIV, Frequently Cited Companies (Abbreviations), and page XV, Country Codes in patent references. The names of periodical publications are abbreviated exactly as done by Chemical Abstracts Service.

abs.	absolute	BAM	Bundesanstalt für Materialprüfung (Federal Republic of Germany)
a.c.	alternating current	BAT	Biologischer Arbeitsstoff-Toleranz-Wert (biological tolerance value for a working material, established by MAK Commission, see MAK)
ACGIH	American Conference of Governmental Industrial Hygienists	Beilstein	Beilstein's Handbook of Organic Chemistry, Springer, Berlin – Heidelberg – New York
ACS	American Chemical Society	BET	Brunauer – Emmett – Teller
ADI	acceptable daily intake	BGA	Bundesgesundheitsamt (Federal Republic of Germany)
ADN	accord européen relatif au transport international des marchandises dangereuses par voie de navigation interieure (European agreement concerning the international transportation of dangerous goods by inland waterways)	BGBI.	Bundesgesetzblatt (Federal Republic of Germany)
ADNR	ADN par le Rhin (regulation concerning the transportation of dangerous goods on the Rhine and all national waterways of the countries concerned)	BIOS	British Intelligence Objectives Subcommittee Report (see also FIAT)
ADP	adenosine 5'-diphosphate	BOD	biological oxygen demand
ADR	accord européen relatif au transport international des marchandises dangereuses par route (European agreement concerning the international transportation of dangerous goods by road)	<i>bp</i>	boiling point
AEC	Atomic Energy Commission (United States)	B.P.	British Pharmacopeia
a.i.	Active ingredient	BS	British Standard
AICHe	American Institute of Chemical Engineers	ca.	circa
AIME	American Institute of Mining, Metallurgical, and Petroleum Engineers	calcd.	calculated
ANSI	American National Standards Institute	CAS	Chemical Abstracts Service
AMP	adenosine 5'-monophosphate	cat.	catalyst, catalyzed
APhA	American Pharmaceutical Association	CEN	Comité Européen de Normalisation
API	American Petroleum Institute	cf.	compare
ASTM	American Society for Testing and Materials	CFR	Code of Federal Regulations (United States)
ATP	adenosine 5'-triphosphate	cfu	colony forming units
		Chap.	chapter
		ChemG	Chemikaliengesetz (Federal Republic of Germany)
		C.I.	Colour Index
		CIOS	Combined Intelligence Objectives Subcommittee Report (see also FIAT)
		CNS	central nervous system
		Co.	Company
		COD	chemical oxygen demand
		conc.	concentrated
		const.	constant
		Corp.	Corporation
		crit.	critical

CTFA	The Cosmetic, Toiletry and Fragrance Association (United States)	FIAT	Field Information Agency, Technical (United States reports on the chemical industry in Germany, 1945)
DAB 9	Deutsches Arzneibuch, 9th ed., Deutscher Apotheker-Verlag, Stuttgart 1986	Fig.	figure
d.c.	direct current	<i>fp</i>	freezing point
decomp.	decompose, decomposition	Friedländer	P. Friedländer, Fortschritte der Teerfarbenfabrikation und verwandter Industriezweige, Vol. 1 – 25, Springer, Berlin 1888 – 1942
DFG	Deutsche Forschungsgemeinschaft (German Science Foundation)	FT	Fourier transform
dil.	dilute, diluted	(g)	gas, gaseous
DIN	Deutsche Industrie Norm (Federal Republic of Germany)	GC	gas chromatography
DMF	dimethylformamide	GefStoffV	Gefahrstoffverordnung (regulations in the Federal Republic of Germany concerning hazardous substances)
DNA	deoxyribonucleic acid	GGVE	Verordnung in der Bundesrepublik Deutschland über die Beförderung gefährlicher Güter mit der Eisenbahn (regulation in the Federal Republic of Germany concerning the transportation of dangerous goods by rail)
DOE	Department of Energy (United States)	GGVS	Verordnung in der Bundesrepublik Deutschland über die Beförderung gefährlicher Güter auf der Straße (regulation in the Federal Republic of Germany concerning the transportation of dangerous goods by road)
DOT	Department of Transportation – Materials Transportation Bureau (United States)	GGVSee	Verordnung in der Bundesrepublik Deutschland über die Beförderung gefährlicher Güter mit Seeschiffen (regulation in the Federal Republic of Germany concerning the transportation of dangerous goods by sea-going vessels)
DTA	differential thermal analysis	GLC	gas-liquid chromatography
EC	effective concentration	Gmelin	Gmelin's Handbook of Inorganic Chemistry, 8th ed., Springer, Berlin – Heidelberg – New York
EC	European Community	GRAS	generally recognized as safe
ed.	editor, edition, edited	Hal	halogen substituent (–F, –Cl, –Br, –I)
e.g.	for example	Houben-Weyl	Methoden der organischen Chemie, 4th ed., Georg Thieme Verlag, Stuttgart
emf	electromotive force	HPLC	high performance liquid chromatography
EmS	Emergency Schedule	IAEA	International Atomic Energy Agency
EN	European Standard (European Community)	IARC	International Agency for Research on Cancer, Lyon, France
EPA	Environmental Protection Agency (United States)		
EPR	electron paramagnetic resonance		
Eq.	equation		
ESCA	electron spectroscopy for chemical analysis		
esp.	especially		
ESR	electron spin resonance		
Et	ethyl substituent (–C ₂ H ₅)		
et al.	and others		
etc.	et cetera		
EVO	Eisenbahnverkehrsordnung (Federal Republic of Germany)		
exp (...)	e ^(...) , mathematical exponent		
FAO	Food and Agriculture Organization (United Nations)		
FDA*	Food and Drug Administration (United States)		
FD & C	Food, Drug and Cosmetic Act (United States)		
FHSA	Federal Hazardous Substances Act (United States)		

IATA-DGR	International Air Transport Association, Dangerous Goods Regulations		
ICAO	International Civil Aviation Organization		
i.e.	that is		
i.m.	intramuscular		
IMDG	International Maritime Dangerous Goods Code		
IMO	Inter-Governmental Maritime Consultative Organization (in the past: IMCO)	max.	maximum
Inst.	Institute	MCA	Manufacturing Chemists Association (United States)
i.p.	intraperitoneal	Me	methyl substituent ($-\text{CH}_3$)
IR	infrared	Methodicum	Chimicum Methodicum
ISO	International Organization for Standardization		Chimicum, Georg Thieme Verlag, Stuttgart
IUPAC	International Union of Pure and Applied Chemistry	MFAG	Medical First Aid Guide for Use in Accidents Involving Dangerous Goods
i.v.	intravenous	MIK	maximale Immissionskonzentration (maximum immission concentration)
Kirk-Othmer	Encyclopedia of Chemical Technology, 3rd ed., J. Wiley & Sons, New York – Chichester – Brisbane – Toronto 1978 – 1984; 4th ed., J. Wiley & Sons, New York – Chichester – Brisbane – Toronto 1991 – 1998	min.	minimum
(l)	liquid	mp	melting point
Landolt-Börnstein	Zahlenwerte u. Funktionen aus Physik, Chemie, Astronomie, Geophysik u. Technik, Springer, Heidelberg 1950 – 1980; Zahlenwerte und Funktionen aus Naturwissenschaften und Technik, Neue Serie, Springer, Heidelberg, since 1961	MS	mass spectrum, mass spectrometry
LC ₅₀	lethal concentration for 50 % of the test animals	NAS	National Academy of Sciences (United States)
LCLo	lowest published lethal concentration	NASA	National Aeronautics and Space Administration (United States)
LD ₅₀	lethal dose for 50 % of the test animals	NBS	National Bureau of Standards (United States)
LDLo	lowest published lethal dose	NCTC	National Collection of Type Cultures (United States)
ln	logarithm (base e)	NIH	National Institutes of Health (United States)
LNG	liquefied natural gas	NIOSH	National Institute for Occupational Safety and Health (United States)
log	logarithm (base 10)	NMR	nuclear magnetic resonance
LPG	liquefied petroleum gas	no.	number
M	mol/L	NOEL	no observed effect level
M	metal (in chemical formulas)	NRC	Nuclear Regulatory Commission (United States)
MAK	Maximale Arbeitsplatz-Konzentration (maximum concentration at the workplace in the Federal Republic of Germany); cf. Deutsche Forschungsgemeinschaft (ed.): Maximale Arbeitsplatzkonzentrationen (MAK) und Biologische Arbeitsstoff-Toleranz-Werte (BAT), WILEY-VCH Verlag, Weinheim (published annually)	NRDC	National Research Development Corporation (United States)
		NSC	National Service Center (United States)
		NSF	National Science Foundation (United States)
		NTSB	National Transportation Safety Board (United States)
		OECD	Organization for Economic Cooperation and Development
		OSHA	Occupational Safety and Health Administration (United States)

p., pp.	page, pages		regulation in Federal Republic of Germany)
Patty	G. D. Clayton, F. E. Clayton (eds.): Patty's Industrial Hygiene and Toxicology, 3rd ed., Wiley Interscience, New York	TA Lärm	Technische Anleitung zum Schutz gegen Lärm (low noise regulation in Federal Republic of Germany)
PB	Publication Board Report (U.S. Department of Commerce, Scientific and Industrial Reports)	TDLo	lowest published toxic dose
report		THF	tetrahydrofuran
PEL	permitted exposure limit	TLC	thin layer chromatography
Ph	phenyl substituent ($-\text{C}_6\text{H}_5$)	TLV	Threshold Limit Value (TWA and STEL); published annually by the American Conference of Governmental Industrial Hygienists (ACGIH), Cincinnati, Ohio
Ph. Eur.	European Pharmacopoeia, 2nd. ed., Council of Europe, Strasbourg 1981	TOD	total oxygen demand
phr	part per hundred rubber (resin)	TRK	Technische Richtkonzentration (lowest technically feasible level)
PNS	peripheral nervous system	TSCA	Toxic Substances Control Act (United States)
ppm	parts per million	TÜV	Technischer Überwachungsverein (Technical Control Board of the Federal Republic of Germany)
q. v.	which see (quod vide)	TWA	Time Weighted Average
ref.	refer, reference	UBA	Umweltbundesamt (Federal Environmental Agency)
resp.	respectively	Ullmann	Ullmann's Encyclopedia of Industrial Chemistry, 5th ed., VCH Verlagsgesellschaft, Weinheim, 1985 - 1996; Ullmanns Encyklopädie der Technischen Chemie, 4th ed., Verlag Chemie, Weinheim 1972 - 1984; 3rd ed., Urban und Schwarzenberg, München 1951 - 1970
R_f	retention factor (TLC)	USAEC	United States Atomic Energy Commission
R. H.	relative humidity	USAN	United States Adopted Names
RID	règlement international concernant le transport des marchandises dangereuses par chemin de fer (international convention concerning the transportation of dangerous goods by rail)	USD	United States Dispensatory
RNA	ribonucleic acid	USDA	United States Department of Agriculture
R phrase	risk phrase according to ChemG and GefStoffV (Federal Republic of Germany)	U.S.P.	United States Pharmacopeia
(R-Satz)		UV	ultraviolet
rpm	revolutions per minute	UVV	Unfallverhütungsvorschriften der Berufsgenossenschaft (workplace safety regulations in the Federal Republic of Germany)
RTECS	Registry of Toxic Effects of Chemical Substances, edited by the National Institute of Occupational Safety and Health (United States)	VbF	Verordnung in der Bundesrepublik Deutschland über die Errichtung und den Betrieb von Anlagen zur Lagerung, Abfüllung und Beförderung brennbarer Flüssigkeiten (regulation in the Federal Republic of Germany)
(s)	solid		
SAE	Society of Automotive Engineers (United States)		
s.c.	subcutaneous		
SI	International System of Units		
SIMS	secondary ion mass spectrometry		
S phrase	safety phrase according to ChemG and GefStoffV (Federal Republic of Germany)		
(S-Satz)			
STEL	Short Term Exposure Limit (see TLV)		
STP	standard temperature and pressure (0°C , 101.325 kPa)		
T_g	glass transition temperature		
TA Luft	Technische Anleitung zur Reinhaltung der Luft (clean air		

	concerning the construction and operation of plants for storage, filling, and transportation of flammable liquids; classification according to the flash point of liquids, in accordance with the classification in the United States)	vs.	versus
		WGK	Wassergefährdungsklasse (water hazard class)
		WHO	World Health Organization (United Nations)
VDE	Verband Deutscher Elektroingenieure (Federal Republic of Germany)	Winnacker-Küchler	Chemische Technologie, 4th ed., Carl Hanser Verlag, München, 1982-1986; Winnacker-Küchler, Chemische Technik: Prozesse und Produkte, Wiley-VCH, Weinheim, from 2003
VDI	Verein Deutscher Ingenieure (Federal Republic of Germany)	wt	weight
vol	volume	\$	U.S. dollar, unless otherwise stated
vol.	volume (of a series of books)		

Frequently Cited Companies (Abbreviations)

Air Products	Air Products and Chemicals	ICI	Imperial Chemical Industries
Akzo	Algemene Koninklijke Zout Organon	IFP	Institut Français du Pétrole
Alcoa	Aluminum Company of America	INCO	International Nickel Company
Allied	Allied Corporation	3M	Minnesota Mining and Manufacturing Company
Amer.	American Cyanamid Company	Mitsubishi Chemical	Mitsubishi Chemical Industries
Cyanamid	Cyanamid Company	Monsanto	Monsanto Company
BASF	BASF Aktiengesellschaft	Nippon	Nippon Shokubai Kagaku
Bayer	Bayer AG	Shokubai	Kogyo
BP	British Petroleum Company	PCUK	Pechiney Ugine Kuhlmann
Celanese	Celanese Corporation	PPG	Pittsburg Plate Glass Industries
Daicel	Daicel Chemical Industries	Searle	G.D. Searle & Company
Dainippon	Dainippon Ink and Chemicals Inc.	SKF	Smith Kline & French Laboratories
Dow Chemical	The Dow Chemical Company	SNAM	Società Nazionale Metandotti
DSM	Dutch Staats Mijnen	Sohio	Standard Oil of Ohio
Du Pont	E.I. du Pont de Nemours & Company	Stauffer	Stauffer Chemical Company
Exxon	Exxon Corporation	Sumitomo	Sumitomo Chemical Company
FMC	Food Machinery & Chemical Corporation	Toray	Toray Industries Inc.
GAF	General Aniline & Film Corporation	UCB	Union Chimique Belge
W.R. Grace	W.R. Grace & Company	Union Carbide	Union Carbide Corporation
Hoechst	Hoechst Aktiengesellschaft	UOP	Universal Oil Products Company
IBM	International Business Machines Corporation	VEBA	Vereinigte Elektrizitäts- und Bergwerks-AG
		Wacker	Wacker Chemie GmbH

Country Codes

The following list contains a selection of standard country codes used in the patent references.

AT	Austria	ID	Indonesia
AU	Australia	IL	Israel
BE	Belgium	IT	Italy
BG	Bulgaria	JP	Japan *
BR	Brazil	LU	Luxembourg
CA	Canada	MA	Morocco
CH	Switzerland	NL	Netherlands *
CS	Czechoslovakia	NO	Norway
DD	German Democratic Republic	NZ	New Zealand
DE	Federal Republic of Germany (and Germany before 1949) *	PL	Poland
DK	Denmark	PT	Portugal
ES	Spain	SE	Sweden
FI	Finland	SU	Soviet Union
FR	France	US	United States of America
GB	United Kingdom	YU	Yugoslavia
GR	Greece	ZA	South Africa
HU	Hungary	EP	European Patent Office *
		WO	World Intellectual Property Organization

* For Europe, Federal Republic of Germany, Japan, and the Netherlands, the type of patent is specified: EP (patent), EP-A (application), DE (patent), DE-OS (Offenlegungsschrift), DE-AS (Auslegeschrift), JP (patent), JP-Kokai (Kokai tokkyo koho), NL (patent), and NL-A (application).

Periodic Table of Elements

element symbol, atomic number, and relative atomic mass (atomic weight)

1A "European" group designation and old IUPAC recommendation
1 group designation to 1986 IUPAC proposal
IA "American" group designation, also used by the Chemical Abstracts Service until the end of 1986

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Laboratory Information and Management Systems (LIMS)

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1. Introduction

Laboratory information and management systems (LIMS) support both the administrative tasks of order processing and also the acquisition and assessment of results in the laboratory. LIMS “informs” about results and “manages” order processing.

The laboratory as a production center for discoveries – and so subject to the rules of production planning – is a new and unfamiliar idea. The laboratory is still being recognized as a creative (innovative) work center with a problem-oriented working procedure for nonrecurrent problems. Work of this kind is generally considered to be unpredictable and therefore only plannable to a limited degree. If this was true, however laboratory work could not be combined with the systematic arrangement that supports an information system, and data processing support in the laboratory would only be of minor importance.

In an analytical laboratory, orders and work flow can effectively be dealt with according to a

plan and guidelines. For every laboratory there is a limited, yet established array of services depending on the instrumental equipment, the qualifications of personnel, and the objects to be analyzed.

Orders, samples, and analytical methods can be systematically described by a suitable data model.

Laboratory orders are plannable and can be carried out according to the rules of operations scheduling. The uncertainties of time for laboratory orders are greater for material and methodical reasons compared with production planning. In the laboratory operations scheduling is usually controlled with less attention to particulars. Nevertheless the preconditions exist for a time, capacity, and personnel plan together with those for an order processing procedure supported by data processing. Laboratory information and management systems undertake these tasks.