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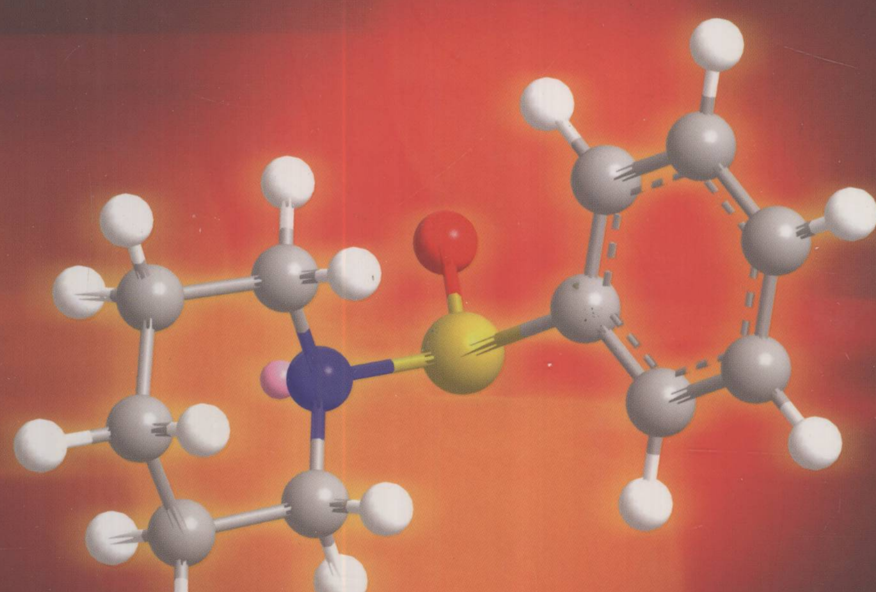
ENCYCLOPEDIA OF REAGENTS FOR ORGANIC SYNTHESIS

SECOND EDITION



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Benzyl Nitrophenyl

Encyclopedia of Reagents for Organic Synthesis

Second Edition

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Volume 1

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Benzyl Nitrophenyl

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General Abbreviations

Ac	acetyl
acac	acetylacetonate
AIBN	2,2′-azobisisobutyronitrile
Ar	aryl
BBN	borabicyclo[3.3.1]nonane
BCME	dis(chloromethyl)ether
BHT	butylated hydroxytoluene (2,6-di-*t*-butyl-*p*-cresol)
BINAL-H	2,2′-dihydroxy-1,1′-binaphthyl-lithium aluminum hydride
BINAP	2,2′-bis(diphenylphosphino)-1,1′-binaphthyl
BINOL	1,1′-bi-2,2′-naphthol
bipy	2,2′-bipyridyl
BMS	borane–dimethyl sulfide
Bn	benzyl
Boc	*t*-butoxycarbonyl
BOM	benzyloxymethyl
bp	boiling point
Bs	brosyl (4-bromobenzenesulfonyl)
BSA	*N,O*-bis(trimethylsilyl)acetamide
Bu	*n*-butyl
Bz	benzoyl
CAN	cerium(IV) ammonium nitrate
Cbz	benzyloxycarbonyl
CDI	*N,N′*-carbonyldiimidazole
CHIRAPHOS	2,3-bis(diphenylphosphino)butane
Chx	=Cy
cod	cyclooctadiene
cot	cyclooctatetraene
Cp	cyclopentadienyl
CRA	complex reducing agent
CSA	10-camphorsulfonic acid
CSI	chlorosulfonyl isocyanate
Cy	cyclohexyl
d	density
DABCO	1,4-diazabicyclo[2.2.2]octane
DAST	*N,N′*-diethylaminosulfur trifluoride
dba	dibenzylideneacetone
DBAD	di-*t*-butyl azodicarboxylate
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DCC	*N,N′*-dicyclohexylcarbodiimide
DCME	dichloromethyl methyl ether
DDO	dimethyldioxirane
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
de	diastereomeric excess
DEAD	diethyl azodicarboxylate
DET	diethyl tartrate
DIBAL	diisobutylaluminum hydride
DIEA	=DIPEA
DIOP	2,3-*O*-isopropylidene-2,3-dihydroxy-1,4-bis-(diphenylphosphino)butane
DIPEA	diisopropylethylamine
diphos	=dppe
DIPT	diisopropyl tartrate
DMA	dimethylacetamide
DMAD	dimethyl acetylenedicarboxylate
DMAP	4-(dimethylamino)pyridine
DME	1,2-dimethoxyethane
DMF	dimethylformamide
dmg	dimethylglyoximato
DMPU	*N,N′*-dimethylpropyleneurea
DMS	dimethyl sulfide
DMSO	dimethyl sulfoxide
DMTSF	dimethyl(methylthio) sulfonium tetrafluoroborate
dppb	1,4-bis(diphenylphosphino)butane
dppe	1,2-bis(diphenylphosphino)ethane
dppf	1,1′-bis(diphenylphosphino)ferrocene
dppp	1,3-bis(diphenylphosphino)propane
DTBP	di-*t*-butyl peroxide
EDA	ethyl diazoacetate
EDC	1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide
EDCI	=EDC
ee	enantiomeric excess
EE	1-ethoxyethyl
Et	ethyl
ETSA	ethyl trimethylsilylacetate
EWG	electron withdrawing group
Fc	ferrocenyl
Fmoc	9-fluorenylmethoxycarbonyl
fp	flash point
Hex	*n*-hexyl
HMDS	hexamethyldisilazane
HMPA	hexamethylphosphoric triamide
HOBt	l-hydroxybenzotriazole
HOBT	=HOBt
HOSu	*N*-hydroxysuccinimide
Im	imidazole (imidazolyl)
Ipc	isopinocampheyl
IR	infrared
KHDMS	potassium hexamethyldisilazide
LAH	lithium aluminum hydride
LD_{50}	dose that is lethal to 50% of test subjects

LDA	lithium diisopropylamide
LDMAN	lithium 1-(dimethylamino)naphthalenide
LHMDS	=LiHMDS
LICA	lithium isopropylcyclohexylamide
LiHMDS	lithium hexamethyldisilazide
LiTMP	lithium 2,2,6,6-tetramethylpiperidide
LTMP	=LiTMP
LTA	lead tetraacetate
lut	lutidine
m-CPBA	*m*-chloroperbenzoic acid
MA	maleic anhydride
MAD	methylaluminum bis(2,6-di-*t*-butyl-4-methylphenoxide)
MAT	methylaluminum bis(2,4,6-tri-*t*-butylphenoxide)
Me	methyl
MEK	methyl ethyl ketone
MEM	(2-methoxyethoxy)methyl
MIC	methyl isocyanate
MMPP	magnesium monoperoxyphthalate
MOM	methoxymethyl
MoOPH	oxodiperoxomolybdenum(pyridine)-(hexamethylphosphoric triamide)
mp	melting point
MPM	=PMB
Ms	mesyl (methanesulfonyl)
MS	mass spectrometry; molecular sieves
MTBE	methyl *t*-butyl ether
MTM	methylthiomethyl
MVK	methyl vinyl ketone
n	refractive index
NaHDMS	sodium hexamethyldisilazide
Naph	naphthyl
NBA	*N*-bromoacetamide
nbd	norbornadiene (bicyclo[2.2.1]hepta-2,5-diene)
NBS	*N*-bromosuccinimide
NCS	*N*-chlorosuccinimide
NIS	*N*-iodosuccinimide
NMO	*N*-methylmorpholine *N*-oxide
NMP	*N*-methyl-2-pyrrolidinone
NMR	nuclear magnetic resonance
NORPHOS	bis(diphenylphosphino)bicyclo[2.2.1]-hept-5-ene
Np	=Naph
PCC	pyridinium chlorochromate
PDC	pyridinium dichromate
Pent	*n*-pentyl
Ph	phenyl
phen	1,10-phenanthroline
Phth	phthaloyl
Piv	pivaloyl
PMB	*p*-methoxybenzyl
PMDTA	*N,N,N′,N″,N″*-pentamethyldiethylenetriamine
PPA	polyphosphoric acid
PPE	polyphosphate ester
PPTS	pyridinium *p*-toluenesulfonate
Pr	*n*-propyl
PTC	phase transfer catalyst/catalysis
PTSA	*p*-toluenesulfonic acid
py	pyridine
RAMP	(R)-1-amino-2-(methoxymethyl)pyrrolidine
rt	room temperature
salen	bis(salicylidene)ethylenediamine
SAMP	(*S*)-1-amino-2-(methoxymethyl)pyrrolidine
SET	single electron transfer
Sia	siamyl (3-methyl-2-butyl)
TASF	tris(diethylamino)sulfonium difluorotrimethylsilicate
TBAB	tetrabutylammonium bromide
TBAF	tetrabutylammonium fluoride
TBAD	=DBAD
TBAI	tetrabutylammonium iodide
TBAP	tetrabutylammonium perruthenate
TBDMS	*t*-butyldimethylsilyl
TBDPS	*t*-butyldiphenylsilyl
TBHP	*t*-butyl hydroperoxide
TBS	=TBDMS
TCNE	tetracyanoethylene
TCNQ	7,7,8,8-tetracyanoquinodimethane
TEA	triethylamine
TEBA	triethylbenzylammonium chloride
TEBAC	=TEBA
TEMPO	2,2,6,6-tetramethylpiperidinoxyl
TES	triethylsilyl
Tf	triflyl (trifluoromethanesulfonyl)
TFA	trifluoroacetic acid
TFAA	trifluoroacetic anhydride
THF	tetrahydrofuran
THP	tetrahydropyran; tetrahydropyranyl
Thx	thexyl (2,3-dimethyl-2-butyl)
TIPS	triisopropylsilyl
TMANO	trimethylamine *N*-oxide
TMEDA	*N,N,N′,N′*-tetramethylethylenediamine
TMG	1,1,3,3-tetramethylguanidine
TMS	trimethylsilyl
Tol	*p*-tolyl
TPAP	tetrapropylammonium perruthenate
TBHP	*t*-butyl hydroperoxide
TPP	tetraphenylporphyrin
Tr	trityl (triphenylmethyl)
Ts	tosyl (*p*-toluenesulfonyl)
TTN	thallium(III) nitrate
UHP	urea–hydrogen peroxide complex
Z	=Cbz

Encyclopedia of Reagents for Organic Synthesis

Second Edition

Encyclopedia of Reagents for Organic Synthesis (EROS)

founded by

Leo A. Paquette

A Range of Products Designed for the Synthetic Chemist

e-EROS

This is the online version of *EROS*, an evolving reference work and database containing detailed and comprehensive information on a wide range of reagents and catalysts.

e-EROS is updated and expanded each year with approximately 200 new and updated reagents and catalysts, and allows for sophisticated reaction, structure and sub-structure searches. It enables the user to make best use of HTML functionality for searching, linking and cross-referencing, while the planned introduction of PDF files will make for comfortable reading and printing. For more information visit www.wiley.com.

EROS Second Edition (EROS II)

This 14-volume work, which you are now browsing, has been substantially expanded since the 8-volume first edition was published in 1995. It includes all the reagents and catalysts that have been published online in *e-EROS* as at the date of publication. It systematically lists and details over 4000 reagents and catalysts and includes detailed indexes in Volume 14 to allow you to find the information you require among the wealth of high-quality content. This new print edition is a landmark publication in the field of organic synthesis and is a must for any major library proud of its range of print publications.

Handbooks for Reagents in Organic Synthesis

These one-volume handbooks are intended to be used on a day-to-day basis by practicing synthetic chemists working in the laboratory. Each volume focuses on a specific sub-set of reagents and catalysts from *e-EROS*, and thereby constitutes a practical, stand-alone tool. Each volume includes a general introduction and list of selected monographs and reviews specific to the particular topic being addressed. Recently published handbooks have covered the following topics: Radical and Radical Ion Chemistry, Catalyst Components for Coupling Reactions, Fluorine-Containing Reagents and Direct Functionalization for C–H Bonds. For a complete list of available handbooks consult www.wiley.com.

e-EROS and its derived products are indispensable sources of information for everybody working in organic synthesis!

Editorial Board

Preface to the First Edition

The extent to which organic synthetic methodology has developed and flourished during the past several decades has placed unusually heavy demands on the broad range of scientists who utilize chemical reagents. There exists the vital need to know which reagent will perform a specific transformation. Since a number of reagents are often amenable to similar objectives, a researcher's ability to access readily a comparative summary of those features that distinguish one reagent from another can result in a considerable economy of time. The purpose of the *Encyclopedia of Reagents for Organic Synthesis* is to incorporate into a single work a genuinely authoritative and systematic description of the utility of all reagents used in organic chemistry. Its comprehensiveness is further served by an unrivaled ease to locate any specific entry or topic. These objectives have been met by inviting practicing chemists from throughout the world to provide specific contributions in their area of expertise. Furthermore, the masthead for each of the 3000 reagents provides valuable information concerning physical data, solubility, form supplied in, purification, and, where relevant, preparative methods. The CAS registry number, handling/storing information, and precautions will further serve potential users. The first literature reference in each entry provides reviews, if available, dealing with the subject reagent. The critical coverage of all relevant literature is extensive. The goal of the *Encyclopedia of Reagents for Organic Synthesis* is to serve as a reference work where the retrievability of useful information concerning any specific reagent is made facile. For this reason there is a detailed subject index and, in addition, a formula index of all the reagents.

In any undertaking of this type, it is important that the term 'reagent' be clearly defined. The guideline that has dominated the thinking of the members of the Editorial Board is that a reagent be an agent or a combination of agents which with some generality effects the transformation of a substrate into a product. In addition, many useful building blocks have been included. As a consequence, we anticipate that a work has been produced that will serve biochemists, material scientists, pharmacologists, and chemical engineers, in addition to chemists from all disciplines, in that manner most conducive to accelerating progress in their respective fields of research.

The entries highlight the various uses characteristic of each reagent, with specific examples illustrative of these chemical reactions. The contributions are organized alphabetically and the cross-referencing to other reagents is liberal. Thus, a concerted effort has been made to bring together in one place a detailed compilation of the uses of those reagents that will serve both the beginning and experienced investigator. The wealth of facts contained within the *Encyclopedia of Reagents for Organic Synthesis* has been assimilated in a manner that will cause all scientists to want this source of information kept in close proximity to their laboratory.

A work of this magnitude could not have been brought to realization without the input of a great deal of time, effort, and dedication on the part of a large number of highly responsible individuals. I am especially indebted to the editors – Steven Burke, Robert Coates, Rick Danheiser, Scott Denmark, David Hart, Lanny Liebeskind, Dennis Liotta, Anthony Pearson, Hans Reich, James Rigby, and William Roush – for their tremendously valuable enthusiasm, intensive work, and unstinting persistence. A most critical role has been played by Colin Drayton, not only in conceiving the project but also as a consequence of his range of knowledge of the publishing business in steering us continually in the proper direction and in overseeing the massive editing operation. James Edwards and Mark Volmer are also to be thanked for their central role as assistant section editors. The body of this encyclopedia was composed by over 1000 authors from 40 countries around the world. The knowledge and expertise contributed by these experienced investigators in the form of authoritative treatises dealing with reagents with which they are thoroughly familiar constitutes the scientific underpinning of the entire undertaking. The enlightening end product of their contributions will have a major impact on the conduct of research in organic chemistry and I thank each of these individuals for their insightful entries.

The large contingent of organic chemists alluded to above, directly and indirectly, expects the *Encyclopedia of Reagents for Organic Synthesis* to play a vital role in stimulating creative research in organic chemistry in the years immediately ahead. All of us hope that you will share in this excitement by perusing its many pages and creatively adapting the valuable information contained therein.

Leo A. Paquette
The Ohio State University
Columbus, OH, USA

Preface to the Second Edition

This multivolume reference work is an extensively expanded counterpart of the *Encyclopedia of Reagents for Organic Synthesis (EROS)*, which was introduced to the international chemical community in 1995. At the time, we were very fortunate to have a highly experienced and expert editorial team of organic chemists to enlist responsible authors to help us reach our high-level objectives. The end result was a most serviceable compilation of 3000 reagents, with each entry detailing valuable handling information and physical properties, in addition to key chemical transformations. In the intervening years, a vast array of additional important reagents have been identified and new editors have facilitated the inclusion of updates where warranted, as well as the introduction of new types of entities such as polymer-supported reagents, reagents for peptide synthesis, new catalyst types, and more.

I would like to express my thanks to the current members of the *EROS II* team, David Crich, Philip L. Fuchs and Gary A. Molander for their invaluable contributions to this second edition. In particular, I wish to extend appreciation to Louise Portsmouth from John Wiley & Sons, for her invaluable efforts to maintain order at every stage of the publication process, and to the production team, Fiona Cowie, Louise Rush, Dan Finch and Geoff Reynolds, for the amount of work they put into the production of this encyclopedia, which totals more than 12 000 pages.

I'd like to draw your attention to the manner in which the updates have been incorporated, whereby the most recent entry follows immediately after the original contribution, with illustrative equations and relevant reference citations. This arrangement is anticipated to be of maximum help to the inquiring researcher, with the proximity of the data intended to smooth the way to obtaining the desired information.

Effort has also been put into improving other aspects of presentation. Abbreviated references are no longer being utilized in favor of a more conventional format, plus InChIs and InChiKeys have been introduced just below the CAS numbers, in order to facilitate connections to other databases. Those readers unfamiliar with this identifier system are referred to the article by Stephen R. Heller and Alan D. McNaught following the Introduction. A listing of authors (see Volume 1) is another new feature that will hopefully prove informative to the user of this work and also make the contributors more visible.

Finally, our efforts to assemble as complete a reference work as possible also extend to the electronic sequel, *e-EROS*. While the online version continues to expand and update at regular intervals, the content of the print edition reflects the state of *e-EROS* as of March, 2009. We hope that the frequent use of either resource will stimulate a continuing flow of new research discoveries and help the users to make best use of the wide range of reagents, catalysts and building blocks in their daily work in the laboratory.

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Introduction

The first edition of the *Encyclopedia of Reagents for Organic Synthesis (EROS)* listed approximately 3000 reagents, catalysts, and building blocks. More than 20% of these have been updated for the new edition, *EROS II*, and in order to keep up with the development of organic synthesis, over 1000 new compounds have been added. These new reagents, catalysts, and building blocks reflect the progress made in areas such as organometallic catalysis, cross-coupling reactions, polymer-supported reagents, and click chemistry.

EROS II comprehensively covers in excess of 4000 reagents, catalysts, and building blocks, sorted in alphabetical order. Systematic nomenclature has been used as the standard, but in a few cases, simplified names are used, e.g. Fluorous DEAD or (*R,S*)-CAMPHOS. All articles are self-contained and the use of ***bold italics*** within each article indicates other reagents that have their own entries in the encyclopedia. Further, lists of related reagents are given at the end of most articles.

EROS II, the print edition, is based on the online version of the encylopedia, *e-EROS*. The content of the print edition mirrors the content of the online edition as of mid-March 2009. *e-EROS* will continue to expand beyond this date with regular content updates, and continues to be the major reference source to research reagents or catalysts. In addition to reaction, structure and substructure searching, *e-EROS* offers a wide range of online tools, such as reference links and cross-referencing.

Most articles are devoted to a single reagent, although in some cases, closely related reagents or reagent families are covered under one heading, e.g. Methyl Trimethylsilylacetate is discussed in the article on Ethyl Trimethylsilylacetate, and Lithium Trimethoxyaluminum Hydride in the article on Lithium Tri-*tert*-butoxyaluminum Hydride.

Wherever possible InChI and InChIKeys have been added below the CAS numbers. Both these identifiers have been developed by IUPAC and can be used in printed and electronic data sources, enabling easier linking to other data compilations. More information on these identifiers can be found on page *xvii*, where the trademark for these identifiers is acknowledged; it is not repeated throughout the work. There are some cases where the CAS numbers and/or InChI and InChIKeys do not exist, e.g. polymer-supported reagents or catalysts.

A particular reagent can be found either directly, by going to the appropriate place in the encyclopedia, or from the Subject Index in Volume 14, which includes numerous other topics, such as types of reactions, named reactions, named reagents, general substrates or products, and specific substrates or products. Volume 14 also contains a Reagent Formula Index, listing all reagents and catalysts covered in the encyclopedia.

The IUPAC International Chemical Identifier (InChI^{TM})

The properties and behavior of chemical substances are generally interpreted and discussed in terms of their molecular structures. Chemists use diagrammatic representations to convey structural information, supplemented by verbal descriptions of structure, and conventional chemical nomenclature was developed as a means of specifying a chemical structure in words. Systematic nomenclature provides an unambiguous description of a structure, a diagram of which can be reconstructed from its systematic name. However, there are other means of specifying molecular structures, and those based on 'connection tables' (coded specifications of atomic connectivities) are more suitable than conventional nomenclature for processing by computer, as they are matrix representations of molecular graphs readily governed and handled by graph theory. In parallel with its continued development of verbal nomenclature, IUPAC has developed a structural identifier that can be readily interpreted by computers, or more precisely, by computer algorithms.

The IUPAC International Chemical Identifier (InChI^{TM}) is a freely available, non-proprietary identifier for chemical substances that can be used in both printed and electronic data sources. It is generated from a computerized representation of a molecular structure diagram, which can be produced by chemical structure-drawing software. Its use enables linking of diverse data compilations and unambiguous identification of chemical substances. A full description of the Identifier and software for its generation are available from the IUPAC website,[1] and a helpful compilation of answers to frequently asked questions has been put together at the Unilever Centre for Molecular Science Informatics.[2] A full account of the InChI^{TM} project is in preparation.[3] Commercial structure-drawing software that will generate the Identifier is available from several organizations, listed on the IUPAC website.[1]

The conversion of structural information to the Identifier is based on a set of IUPAC structure conventions, and rules for normalization and canonicalization (conversion to a single, predictable sequence) of an input structure representation. The resulting InChI is simply a series of characters that serve to uniquely identify the structure from which it was derived. This conversion of a graphical representation of a chemical substance into the unique InChI character string can be carried out automatically by any organization, and the facility can be built into any program dealing with chemical structures.

The InChI uses a layered format to represent all available structural information relevant to compound identity. InChI layers are listed below. Each layer in an InChI representation contains a specific type of structural information. These layers, automatically extracted from the input structure, are designed so that each successive layer adds additional detail to the Identifier. The specific layers generated depend on the level of structural detail available and whether or not allowance is made for tautomerism. Of course, any ambiguities or uncertainties in the original structure will remain in the InChI.

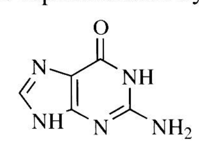
This layered structure design offers a number of advantages. If two structures for the same substance are drawn at different levels of detail, the one with the lower level of detail will, in effect, be contained within the other. Specifically, if one substance is drawn with stereo-bonds and the other without, the layers in the latter will be a subset of the former. The same will hold for compounds treated by one author as tautomers and by another as exact structures with all H-atoms fixed. This can work at a finer level. For example, if one author includes double bond and tetrahedral stereochemistry, but another omits stereochemistry, the latter InChI will be contained in the former.

The InChI layers are:

1. Formula
2. Connectivity (no formal bond orders)
    a. disconnected metals
    b. connected metals
3. Isotopes
4. Stereochemistry
    a. double bond (*Z/E*)
    b. tetrahedral (sp^3)
5. Tautomers (on or off)

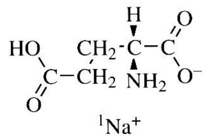
Charges are not part of the basic InChI, but rather are added at the end of the InChI string.

Two examples of InChI representations are given below. It is important to recognize, however, that InChI strings are intended for use by computers and end users need not understand any of their details. In fact, the open nature of InChI and its flexibility of representation, after implementation into software systems, may allow chemists to be even less concerned with the details of structure representation by computers.



guanine

InChI = 1/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)/f/h8,10H,6H2



monosodium glutamate

InChI = 1/C5H9NO4.Na/c6-3(5(9)10)1-2-4(7)8;/h3H,1-2,6H2,(H,7,8)(H,9,10);/q;+1/p-1/t3-;/m1./s1/fC5H8NO4.Na/h7H;/q-1;m

The layers in the InChI string are separated by the '/' character followed by a lowercase letter (except for the first layer, the chemical formula), with the layers arranged in predefined order. In the examples the following segments are included:

InChI version number
/ chemical formula
/c connectivity-1.1 (excluding terminal H)
/h connectivity-1.2 (locations of terminal H, including mobile H attachment points)
/q charge
/p proton balance
/t sp^3 (tetrahedral) parity
/m parity inverted to obtain relative stereo (1 = inverted, 0 = not inverted)
/s stereo type (1 = absolute, 2 = relative, 3 = racemic)
/f chemical formula of the fixed-H structure if it is different
/h connectivity-2 (locations of fixed mobile H)
/q charge
/t sp^3 (tetrahedral) parity
/m parity inverted to obtain relative stereo (1 = inverted, 0 = not inverted, . = inversion does not affect the parity)
/s stereo type (1 = absolute, 2 = *relative*, 3 = racemic)

One of the most important applications of the InChI is the facility to locate mention of a chemical substance using internet-based search engines. This is made easier by using a shorter (compressed) form of InChI, known as the InChIKey.

The InChIKey is a 25-character representation that, because it is compressed, cannot be reconverted into the original structure, but it is not subject to the undesirable and unpredictable breaking of longer character strings by some search engines. An example is shown in Figure 1 below.

The use of the InChIKey also allows searches based solely on atomic connectivity (first 14 characters). Software for generating InChIKey is available from the IUPAC website.[1]

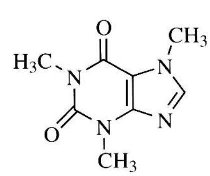
The enormous databases compiled by organizations such as PubChem,[4] the US National Cancer Institute, and ChemSpider[5] contain millions of InChIs and InChIKeys, which allow sophisticated searching of these collections. PubChem provides InChI-based structure-search facilities (for both identical and similar structures),[6] and ChemSpider offers both search facilities and web services enabling a variety of InChI and InChIKey conversions.[7] The NCI Chemical Structure Lookup Service[8] provides InChI-based search access to over 39 million chemical structures from over 80 different public and commercial data sources.

In the age of the computer, the IUPAC International Chemical Identifier is an essential component of the chemist's armory of information tools, enabling location and manipulation of chemical data with unprecedented ease and precision.

Stephen R. Heller and Alan D. McNaught

References

[1] http://www.iupac.org/inchi.
[2] http://wwmm.ch.cam.ac.uk/inchifaq/
[3] *Pure Appl. Chem.*, in preparation.
[4] http://pubchem.ncbi.nlm.nih.gov
[5] http://www.chemspider.com
[6] http://pubchem.ncbi.nlm.nih.gov/search
[7] http://www.chemspider.com/InChI.asmx
[8] http://cholla.chemnavigator.com/cgi-bin/lookup/new/search



InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3 (caffeine)

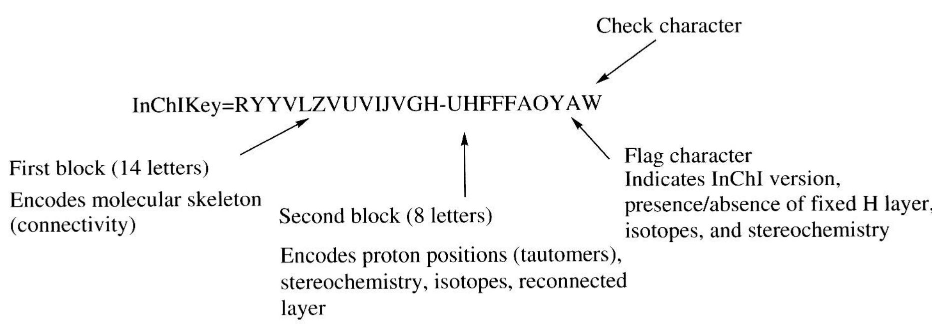


Figure 1 Description of an InchIKey.

Complete List of Contributors

Note: Contributions to the *Encyclopedia of Reagents for Organic Synthesis, Second Edition*, were made at regular intervals between 1994 and 2008. The following section lists the affiliations of contributors at the time of the submission of each article. Some contributors may have changed their affiliation since the original publication of their article and may also have several affiliations reflecting their career development.

Mona Aasmul	*Wayne State University, Detroit, MI, USA*	
	• 2,2-Dimethoxy-5,5-dimethyl-Δ^3-1,3,4-oxadiazoline	3996
Ahmed F. Abdel-Magid	*Johnson & Johnson Pharmaceutical Research & Development, LLC, Spring House, PA, USA*	
	• Sodium Triacetoxyborohydride	8970
	The R. W. Johnson Pharmaceutical Research Institute, Spring House, PA, USA	
	• Barium Hydroxide	420
	• Lithium Hydroxide	6226
	• Potassium Hydroxide	8235
	• Potassium Hydroxide–Alumina	8238
	• Potassium Hydroxide–Carbon Tetrachloride	8239
	• Potassium Hydroxide–18-Crown-6	8240
	• Potassium Hydroxide–Dimethyl Sulfoxide	8242
	• Potassium Hydroxide–Hexamethylphosphoric Triamide	8243
Andrew Abell	*University of Canterbury, Christchurch, New Zealand*	
	• Dimethyl Bis(methylthio)methylphosphonate	4096
	• Dimethyl Methylphosphonate	4225
	• Triethyl Phosphonoacetate	9945
	• Trimethyl Phosphonoacetate	10280
K. Abiraj	*University of Mysore, Mysore, India*	
	• Ammonium Formate	348
Ahmed I. Abouelatta	*Wayne State University, Detroit, MI, USA*	
	• Chlorotris(diethylamino)titanium	2518
José Luis Aceña	*Centro de Investigación Principe Felipe, Valencia, Spain*	
	• Trifluoroiodomethane	10009
	• Trifluoromethyltrimethylsilane	10107
Waldemar Adam	*University of Würzburg, Würzburg, Germany*	
	• Bis(trimethylsilyl) Monoperoxysulfate	1343
Christopher M. Adams	*Novartis Institutes for Biomedical Research, Cambridge, MA, USA*	
	• 2-(Trimethylsilyl)ethoxymethyl Chloride	10365
Edward J. Adams	*E. I. DuPont de Nemours & Co., Newark, DE, USA*	
	• Cyclopropylidenetriphenylphosphorane	2967
	• Cyclopropyltriphenylphosphonium Bromide	2971
	• Dimethyl(methylthio)sulfonium Tetrafluoroborate	4229
	• 2-Pyridinesulfenyl Bromide	8457
	• Pyridinethiol	8460
Jan A. R. Adams	*ARIAD Pharmaceuticals, Inc., Cambridge, MA, USA*	
	• Trimethylsilylketene	10379
Matthew S. Addie	*University of York, York, UK*	
	• Poly[4-(diacetoxyiodo)styrene]	8073

Javier Adrio	*Universidad Autónoma de Madrid, Madrid, Spain*	
	• Potassium Dichromate	8152
	• Potassium Permanganate	8271
	• Potassium Superoxide	8301
Carlos A. M. Afonso	*Instituto Superior Técnico, Lisbon, Portugal*	
	• Potassium Ferricyanide	8178
David J. Ager	*The NutraSweet Company, Mount Prospect, IL, USA*	
	• Dichlorodimethylsilane	3437
	• Ethyl Lithio(trimethylsilyl)acetate	4975
	• Ethyl Trimethylsilylacetate	5029
	• Phenoxyacetic Acid	7751
	• Trimethylsilylacetic Acid	10291
	• Trimethylsilylmethyllithium	10397
	• Trimethylsilylmethylmagnesium Chloride	10400
	• Trimethylsilylmethylpotassium	10408
	DSM, Raleigh, NC, USA	
	• Trimethylsilylmethyllithium	10397
Poonam Aggarwal	*The University of Toledo, Toledo, OH, USA*	
	• Tetracyanoethylene	9179
Varinder K. Aggarwal	*University of Bristol, Bristol, UK*	
	• Dimethylsulfonium Methylide	4307
	• Dimethylsulfoxonium Methylide	4336
	• Trimethylsulfoxonium Iodide	10501
Enrique Aguilar	*Universidad de Oviedo, Oviedo, Spain*	
	• Sodium Periodate	8921
	• Titanium(IV) Chloride	9526
	• Titanium Tetraisopropoxide	9575
	• Trimethylsilyl Trifluoromethanesulfonate	10466
Hubertus Ahlbrecht	*Justus-Liebig University, Giessen, Germany*	
	• Dimethylaminomethyllithium	4068
M. Syarhabil Ahmad	*University of Wisconsin-Milwaukee, Milwaukee, WI, USA*	
	• Bis(cyclopentadienyl)dimethyltitanium	931
Omar K. Ahmad	*Massachusetts Institute of Technology, Cambridge, MA, USA*	
	• Benzenesulfonic Acid, 2-Nitro-, (1-Methylethylidene)hydrazide	509
Jung-Mo Ahn	*The University of Texas at Dallas, Richardson, TX, USA*	
	• Acrylic Acid	123
	• 2-Chloroacrylonitrile	2207
Kenichi Akaji	*Osaka University, Osaka, Japan*	
	• 2-Chloro-1,3-dimethylimidazolidium Hexafluorophosphate	2310
Takahiko Akiyama	*Gakushuin University, Tokyo, Japan*	
	• Dinaphtho[2,1-*d*:1′,2′-*f*][1,3,2]dioxaphosphepin, 4-Hydroxy-2,6-diphenyl-, 4-Oxide, (11b*R*)- (Family of Reagents)	4380
Irini Akritopoulou-Zanze	*University of Southern California, Los Angeles, CA, USA*	
	• Methyltitanium Trichloride	7074
	• Methyltitanium Triisopropoxide	7076
	• Methyltitanium Tris(diethylamide)	7082
Mouâd Alami	*Ecole Normale Supérieure, Paris, France*	
	• 1,2-Dichloroethylene	3448
	• Isopropenyllithium	5871
	• Isopropenylmagnesium Bromide	5883
	• 1-Propenyl Bromide	8395
	• 1-Propenyllithium	8396
	• Vinylmagnesium Bromide	10828

Contributor Affiliations Correct at the Time of Writing

	Université Pierre et Marie Curie, Paris, France	
	• Manganese Dioxide	6378
Fernando Albericio	*Millipore Corporation, Bedford, MA, USA*	
	• Azidotris(dimethylamino)phosphonium Hexafluorophosphate	400
	• 1,1′-Azobis-1-cyclohexanenitrile	404
	• 1-Benzotriazolyl Diethyl Phosphate	554
	• *O*-Benzotriazol-1-yl-*N,N,N′,N′*-tetramethyluronium Hexafluorophosphate	566
	• 4,4′-Bis(2-amino-6-methylpyrimidyl) Disulfide	812
	• 1-Phenylsulfonyl-1*H*-tetrazole	7908
	University of Barcelona, Barcelona, Spain	
	• 4-Bromomethyl-3-nitrobenzoic Acid Linker	1631
	• 2,4-Dimethoxy-4′-hydroxybenzophenone	4005
	• *N*-[(Dimethylamino)-1*H*-1,2,3-triazolo[4,5-*b*]pyridin-1-ylmethylene]-*N*-methylmethanaminium Hexafluorophosphate *N*-Oxide	4086
	• *N*-[9-(Hydroxymethyl)-2-fluorenyl]succinamic Acid	5512
	• 4-Hydroxymethyl-3-nitrobenzoic Acid	5518
	• 3-Hydroxy-3*H*-1,2,3-triazolo[4,5-*b*]pyridine	5575
	• Merrifield Resin	6458
Dino Alberico	*Alphora Research Inc., Mississauga, Ontario, Canada*	
	• Bicyclo[2.2.1]hept-2-ene (Norbornene)	712
Jeffrey S. Albert	*University of Pittsburgh, Pittsburgh, PA, USA*	
	• 1,3-Dicyclohexylcarbodiimide	3557
	• 1,3-Dicyclohexylcarbodiimide–4-Dimethylaminopyridine	3561
Kim F. Albizati	*University of California, San Diego, La Jolla, CA, USA*	
	• 2-Bromo-1-methylpyridinium Iodide	1634
	• Dibromomethyllithium	3136
	• Dichloromethyllithium	3477
	• 4-Ethylenedioxybutyllithium	4931
	• 2-Lithio-*N,N*-diethylbenzamide	5990
	• 1-Methoxyallyllithium	6589
	• *N*-Methyl-*N,N′*-di-*tert*-butylcarbodiimidium Tetrafluoroborate	6816
	• *N*-Methyl-*N,N′*-dicyclohexylcarbodiimidium Iodide	6819
	• 4-(4′-Methyl-1′-piperazinyl)-3-butyn-2-one	7028
	• 1-Methyl-2(1*H*)-pyridinethione	7045
	• Tribromomethyllithium	9735
	• Trichloromethyllithium	9858
Andrés R. Alcántara	*Complutense University, Madrid, Spain*	
	• Potassium Fluoride on Celite	8188
Roger W. Alder	*University of Bristol, Bristol, UK*	
	• Dimethyliodonium Hexafluoroantimonate	4211
	• Methyltrifluoromethanesulfonate	7103
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	• 1,3-Butadiene	1721
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	• Methyl-2-propanesulfinyl Chloride	7034
Christopher W. Alexander	*Clemson University, Clemson, SC, USA*	
	• Lithium Di-*tert*-butylcuprate	6148
	• Lithium Di-(*E*)-1-propenylcuprate	6197
	• Lithium Di-*p*-tolylcuprate	6200
	Emory University, Atlanta, GA, USA	
	• 1,3-Dicyclohexylcarbodiimide–Copper(I) Chloride	3560
	• Lithium Bis(1-ethoxyvinyl)cuprate	6091
	• Lithium (*Z*)-Bis(2-ethoxyvinyl)cuprate	6092
	• Lithium Bis(1-methoxyvinyl)cuprate	6093

Valérie Alezra	*University of Geneva, Geneva, Switzerland*	
	• (*R*,*R*)-1,2-Diphenyl-1,2-[di(pentafluorophenyl)phosphanoxy]ethane	4450
Florent Allais	*ESPCI, Paris, France*	
	• *N*-(2-Pyridyl)bis(trifluoromethanesulfonimide)	8499
Hussein Al-Mughaid	*Dalhousie University, Halifax, Nova Scotia, Canada*	
	• 4-Penten-1-ol	7708
	• Tetrachlorophthalimide	9166
Diego A. Alonso	*Universidad de Alicante, Alicante, Spain*	
	• 3,5-Bis(trifluoromethyl)acetophenone	1282
	• 3,5-Bis(trifluoromethyl)thiophenol	1304
	• Potassium Tetrachloropalladate(II)	8309
	• 1,3,5-Trifluoro-2-nitrobenzene	10120
Ryan A. Altman	*Massachusetts Institute of Technology, Cambridge, MA, USA*	
	• 1,10-Phenanthroline, 4,7-Dimethoxy	7749
Joseph S. Amato	*Merck Research Laboratories, Rahway, NJ, USA*	
	• *p*-Nitrobenzyl 2-Diazo-3-trimethylsilyloxy-3-butenoate	7315
Ilhwan An	*Michigan State University, East Lansing, MI, USA*	
	• 1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane Bis(tetrafluoroborate)	2356
Denise L. Andersen	*University of British Columbia, Vancouver, British Columbia, Canada*	
	• (*Z*)-4-Iodo-1-(tributylstannyl)but-1-ene	5766
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	• Hexamethyldisilazane	5354
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	• Dimethylaluminum Amide	4042
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	• *S*-(1-Oxido-2-pyridinyl)-1,1,3,3-tetramethylthiouronium Hexafluorophosphate (HOTT)	7478
Paul C. Anderson	*Bio-Méga/Boehringer Ingelheim Research, Laval, Quebec, Canada*	
	• *B*-Bromocatecholborane	1548
	• Bromodimethylborane	1567
Pher G. Andersson	*Uppsala University, Uppsala, Sweden*	
	• 2,2-Bis[2-[4(*S*)-*tert*-butyl-1,3-oxazolinyl]]propane	877
Siegfried Andreae	*Institut für Angewandte Chemie, Berlin-Adlershof, Germany*	
	• 1-Oxa-2-azaspiro[2.5]octane	7457
Peter R. Andreana	*Wayne State University, Detroit, MI, USA*	
	• Bis(acetoxy)tetrabutyldistannoxane	765
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	• Carbon Dioxide	2052
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	• Borane–Ammonia	1405
	• Borane–Pyridine	1418
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	• 1,5-Bis(bromomagnesio)pentane	865
	• Magnesium Ethyl Malonate	6334
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	• 1,4-Dilithiobutane	3947
	• 1,5-Dilithiopentane	3951