

INTRODUCTION TO THE DATABASE

The Chapman & Hall/CRC Chemical Database is a structured database holding information on chemical substances. It includes descriptive and numerical data on chemical, physical and biological properties of compounds; systematic and common names of compounds; literature references; structure diagrams and their associated connection tables. *Dictionary of Inorganic and Organometallic Compounds (DIOC) on CD-ROM* is a subset of this and includes all compounds contained in two of Chapman & Hall/CRC's printed chemical dictionaries, *Dictionary of Inorganic Compounds* (Main Work and Supplements) and *Dictionary of Organometallic Compounds* (Second Edition and Supplements).

COMPOUND SELECTION

In general, DIOC includes the following compounds:

- The elements.
- Binary and ternary compounds including hydrides, halides, oxides, sulfides, selenides, tellurides, nitrides, phosphides, and some non-stoichiometric compounds.
- Simple molecular compounds and their adducts, e.g. CS₂, PF₅.
- Simple and complex oxides including heteropolyanions, e.g. SO₃, BaO, TiO₂, La₂O₃, MgAl₂O₄, and representative silicates.
- Common minerals, where possible included under the corresponding 'nearest pure substance'.
- Important coordination compounds, e.g. amines, phosphines, alkoxy complexes, and major well-characterised bioinorganics.
- Organometallic compounds representative of all important structural types (in the case of ligands with organic substituents, typically the parent member of each series, where known, together with a selection of its homologues).
- Compounds with an established use such as catalysts, starting materials, synthetic reagents, etc.
- Other compounds of particular chemical, structural, biological or historical interest, especially those thought to exhibit unusual bonding characteristics.

DATA PRESENTATION AND ORGANISATION

Derivatives and variants

In the database, closely related compounds are grouped together to form an *entry*. Stereoisomers and derivatives of a parent compound are all listed under one entry. The compounds in the *Dictionary of Inorganic and Organometallic Compounds* are grouped together into over 55,000 entries.

The structure of an entry is shown below.

<p>Entry (parent compound) Derivatives</p> <p>Variants (stereoisomers or other closely-related compounds) Derivatives of the variant</p>
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In a simple entry, there is just one compound, with no derivatives or variants. A composite entry will start with the entry name, then may have:

- one or more derivatives at entry level
- one or more variants of the entry
- one or more derivatives of the variant

Variants are commonly stereoisomers or, in the case of intermetallic compounds, substances having different stoichiometries.

Derivatives may include hydrates, complexes, salts, classic organic derivatives and also the following special categories:

(a) Isotopically labelled compounds

Data on only the most important isotopic variants is included, generally limited to those of hydrogen. Deuterium (^2H) and tritium (^3H) are denoted separately in formulae as atoms D and T respectively and are alphabetically indexed as for other atoms. Data for deuterium oxide (D_2O), for example, will be found within the entry for water.

Information on the most important isotopes for each element is provided within the entry for that element.

(b) Dimeric and oligomeric substances

Where a compound is known in several states of aggregation, these are all included in a single entry which usually refers to the monomer. The empirical formulae of all the oligomeric forms are given as well as all appropriate synonyms, and the compound can therefore readily be traced as the monomer or the oligomer.

Compounds which are known only in dimeric form under normal conditions are entered as such but the hypothetical monomers are included as derivatives to provide the names and formulae of the monomeric forms.

(c) Anions and cations

Entries for ionic substances containing complex ions generally refer to the naked complex cation or anion and the formula, formula weight and CAS Registry Number given for the entry are those of the ion, in agreement with current CAS practice. Salts of the ion with various counterions are then treated as derivatives and the empirical formulae of the more important ones are given.

If a specific salt is considered to be of particular importance, it will be given an entry of its own, but there will be a cross-reference between the entry for the complex ion and the salt. For example, the tetraphenylborates: each salt is an important compound in its own right and there are thus separate entries for sodium tetraphenylborate, potassium tetraphenylborate, etc.

(d) Minerals

Wherever possible, minerals corresponding to synthetic compounds are included within the entry for the synthetic compound, e.g. Zinc Blende and Wurtzite are incorporated into the entry for Zinc Sulfide (ZnS). Only when a mineral is the sole point of interest or unavailable synthetically is it given an entry in its own right.

DATA TYPES

The format of a typical entry is given in Fig. 1, and shows the individual types of data that may be present in an entry.

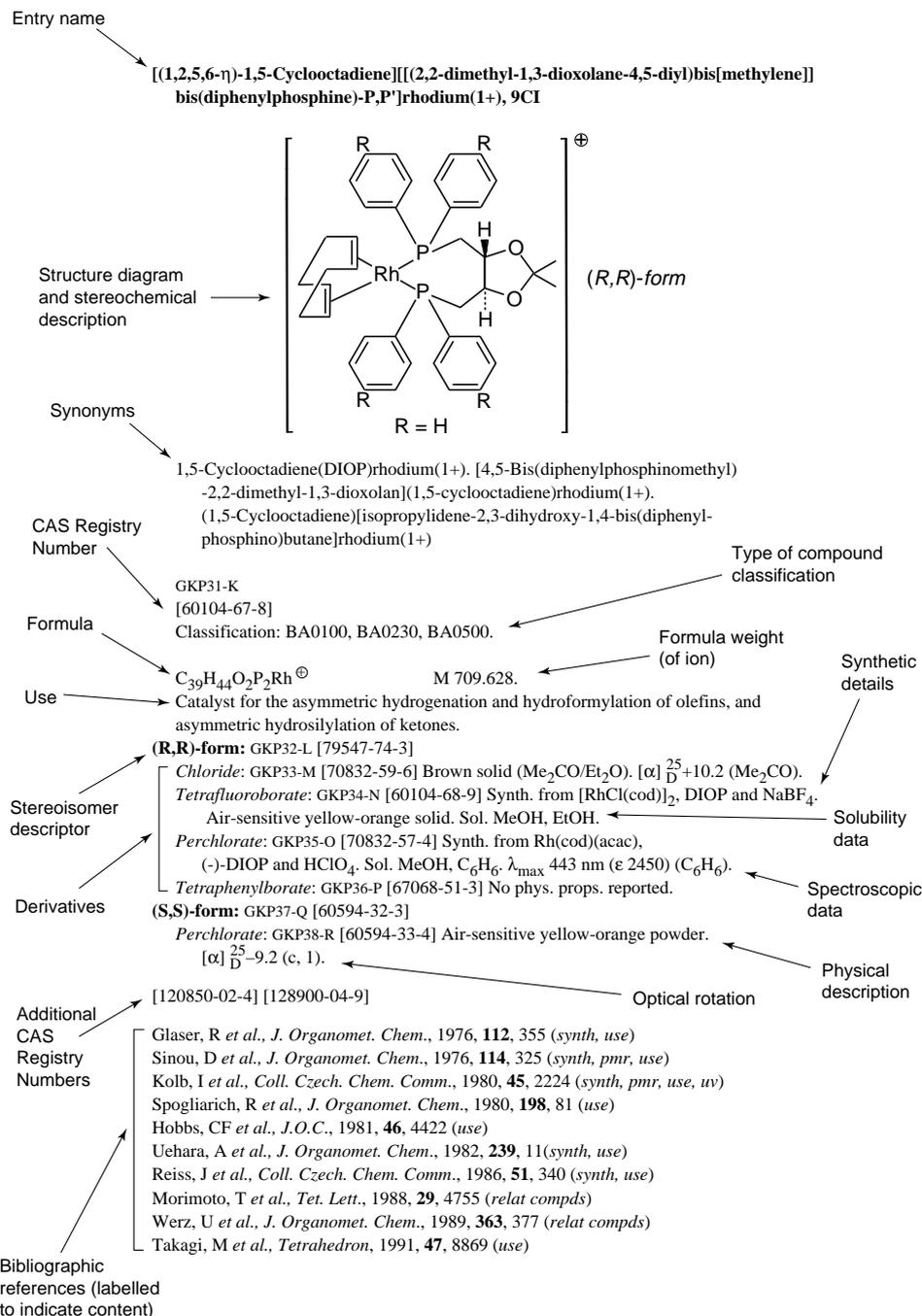


Fig. 1. Sample entry from database

Chemical names and synonyms

All of the names discussed below can be searched using the **Chemical Name** field.

The Entry Name chosen to head each entry is that by which, in the opinion of the editors, it is most likely to be known, and of use to, most users. Systematic names following IUPAC conventions are used wherever convenient, but trivial names may be used for more complex structures. In cases where no one name stands out as being clearly more familiar or convenient than others, the Chemical Abstracts name is normally used as the entry name.

An important function of DIOC is the provision of a wide range of synonyms. In selecting the range of alternative names to present for each compound or derivative, we have been guided by the following principles:

(a) The function of the *Dictionary* is to report names which are found in the literature, including Chemical Abstracts, and not to attempt to impose a system of nomenclature. Therefore the editorial generation of new names has been kept to the minimum required by consistency. The vast majority of names given in DIOC are those given in the original paper(s) and in Chemical Abstracts.

In some cases, two or more non-identical compounds have been given the same trivial name within the chemical literature. Where such a duplication occurs, this is indicated by a dagger symbol (†) immediately following the name.

(b) For compounds of complex structure, such as metal cluster derivatives, only the CAS name is reported. Frequently, the authors of papers reporting such compounds do not attempt to name them and it is to be assumed that most users of DIOC wishing to locate such compounds will do so via the molecular formula.

(c) There are many examples in the primary literature of the naming of inorganic and organometallic compounds which is definitely incorrect according to IUPAC convention, especially in the non-alphabetical ordering of ligands in coordination compounds. Many of these incorrect forms are reported.

(d) Trivial variations in nomenclature which do not materially affect the alphabetical ordering of the name are not included. Such minor variations are legion: a common example is cyclopentadienyl complexes, which may be named as η^5 -cyclopentadienyl, η -cyclopentadienyl (Royal Society of Chemistry practice), η^5 -2,4-cyclopentadien-1-yl (current CAS practice), π -cyclopentadienyl (8CI practice), or h^5 -cyclopentadienyl (older literature).

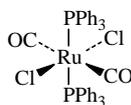
(e) The spellings used for the elements Al, Cs and S in DIOC are aluminium, caesium and sulfur respectively, as recommended by IUPAC.

(f) *CAS names.* Names corresponding to those used by CAS during the 8th through to the 12th Collective Index Periods (1967–71, 1972–76, 1977–81, 1982–86, 1987–1991 respectively) are labelled with the suffixes 8CI, 9CI, 10CI, 11CI and 12CI respectively. Names encountered in CAS since 1991 are labelled 13CI although it is possible that some further changes may have occurred before publication of the 13th Collective Index.

For the majority of inorganic compounds, and simple organometallic compounds such as metal alkyls, the nomenclature brought in for the 9th Collective Index Period (and referred to as 9CI nomenclature) has since been unchanged. This is not true for some groups of compounds such as cluster boranes and the more complex organometallic compounds, where the nomenclature is still evolving. There are also many examples of the same

compound being registered more than once under different names (and registry numbers) in CAS.

The following types of suffix which are to be found attached to CAS names have been omitted. Firstly, stereochemical descriptors, e.g. in Dicarbonyldichlorobis(triphenylphosphine)ruthenium the CAS descriptor (*OC-6-12*) indicates the geometry shown below:



This is referred to in DIOC as the *af*-dicarbonyl-*bd*-dichloro-*ce*-diphosphine form. Secondly, bonding descriptors, e.g. in Hexa- μ -chlorohexachlorotriruthenate(4-) the CAS descriptor (*2Ru-Ru*) denotes the presence of two ruthenium-ruthenium bonds. On the other hand, oxidation state has in many cases been inserted in CAS names. See Section (g) below.

(g) *Oxidation states and charges.* For any given substance, the oxidation state (also known as the Stock number) of the element of interest is incorporated into at least one of the names given, using Roman numerals or zero, provided that it can be unequivocally assigned. Oxidation states are therefore generally omitted from nitrosyl complexes where the assignment of oxidation state is often controversial, and also from compounds of elements having only one common oxidation state, where it is unnecessary.

The overall ionic charge (also known as the Ewens-Bassett number) of a complex is also provided in at least one name, using Arabic numerals.

CAS names do not describe oxidation states, only charges. However, where the CAS name is the only readily accessible one, the oxidation state has been added editorially. Where both oxidation state and charge occur in a single name, the former precedes the latter.

CAS Registry Numbers

CAS Registry Numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by the Chemical Abstracts Service since 1965 (plus retrospective allocation of numbers by CAS to compounds from the sixth and seventh Collective Index Periods). The numbers have no chemical significance but they provide a label for each substance independent of any system of nomenclature.

Much effort has been expended to ensure that accurate CAS numbers are given for as many substances as possible. If a CAS number is not given for a particular compound, it may be (a) because CAS have not allocated one, (b) very occasionally, because an editorial decision cannot be made as to the correct number to cite, or (c) because the substance was added to the DIOC database at a late stage in the compilation process, in which case the number will probably be added to the database soon.

At the foot of the entry, immediately before the references, may be shown additional registry numbers. These are numbers which have been recognised by the Editors or contributors as belonging to the entry concerned but which cannot be unequivocally assigned to any of the compounds covered by the entry. Their main use will be in helping those who need to carry out additional searches, especially online searches in the CAS or other databases, and who will be able to obtain additional hits using these numbers. Clearly, discretion is needed in their use for this purpose.

Additional registry numbers may arise for a variety of reasons:

- (a) A CAS number may refer to stereoisomers or other variants of the main entry compound, e.g. bonding isomers, for which no physical properties or useful information is available. In many cases, although CAS numbers are allocated to different isomers, they are not assigned specifically to each one and are merely labelled 'stereoisomers'.
- (b) Hydrates, salts, complexes, etc. which are not characterised fully.
- (c) A CAS number may refer to a mixture or to a particular non-stoichiometric composition which is not detailed individually in the entry.
- (d) Replaced numbers, duplicate numbers and other numbers arising from CAS indexing procedure or, occasionally, from errors or inconsistencies by CAS, are also reported.

Diagrams

Every attempt has been taken to achieve as much consistency and clarity in the presentation of structural formulae as possible. The primary aim has been to indicate the connectivity and, where known, the stereochemistry.

The diagrams are necessarily stylised and are intended to convey the correct topochemistry rather than to convey accurate representations of bond lengths and angles.

It is a general principle that abbreviations in structural formulae are kept to a minimum and except for very common moieties (e.g. Ph) ligands are drawn out in full.

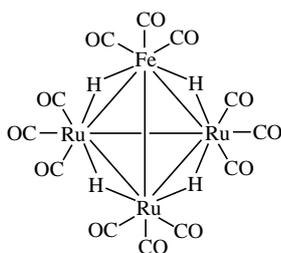
It should be noted that in each entry display there is a single diagram which applies to the parent entry. Separate diagrams are not given for variants or derivatives.

Structures for derivatives can be viewed in **Structure Search**, but remember that these structures are generated from connection tables and may not always be oriented consistently.

Where no structure diagram is given for a particular entry, either the structure of the compound is unknown or the user is referred to the diagram of a related compound via the **Structure by Analogy** keyhole.

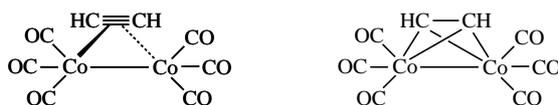
(a) *Bonding*. The bonding in many transition metal complexes and clusters is more or less complex and subject to varying interpretation, and is therefore not amenable to accurate depiction by the conventions which serve reasonably well for organic compounds.

Bridging hydrogens between two metal centres are depicted for clarity as though there are full metal-metal bonds, although there is rarely so much electron density between the two metals, e.g.:



Very considerable variations in conventions for depicting organometallic compounds are to be found in the literature. For example, the two following representations of the complex obtained from octacarbonyldicobalt and

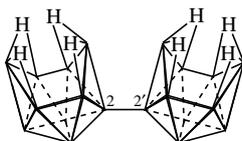
acetylene refer to the same compound:



For sandwich complexes, the following convention, illustrated with ferrocene as an example, is used throughout:



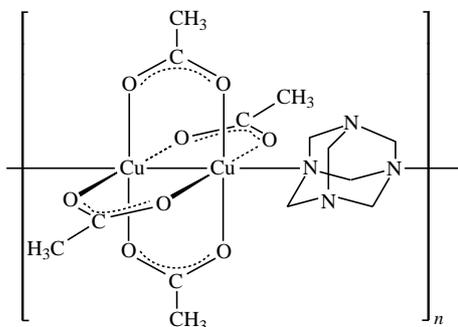
(b) *Boranes*. BH groups in the cluster boranes and related species are represented by vertices, as shown below:



Only when B is bonded to 2 (or more) non-bridging atoms is it depicted explicitly. All other atoms, including carbon, are depicted explicitly.

This convention is analogous to the representation of CH_2 or CH groups as plain vertices in organic compounds and which is also used to depict ligands in this database.

(c) *Polymeric transition metal complexes*. Wherever possible, the coordination polyhedron of the metal is depicted, and the points of attachment to the next unit are indicated using bonds that extend outside square brackets, e.g.:



Stereochemical conventions

Absolute and relative configurations are given according to the (*R,S*)- and (*E,Z*)-conventions wherever feasible.

(a) *The (R,S)-system*

In the simplest case, the four substituent atoms about a tetrahedral carbon atom are placed in order of increasing atomic number and the molecule is then viewed from the side remote from the substituent of lowest priority. The configuration is (*R*) (*rectus*) if the order of the three other groups from highest to lowest is clockwise, and (*S*) (*sinister*) if it is anticlockwise.



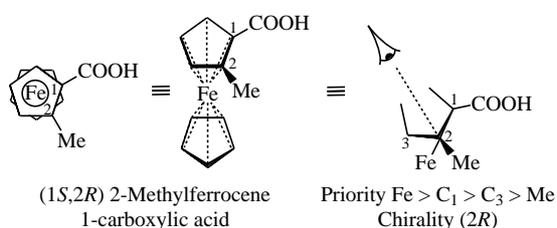
Extensions of the (*R,S*)-system refer to situations such as axial and planar chirality.

Where only the relative configuration of a compound containing more than one chiral centre is known, the symbols (*R**) and (*S**) are used, the lowest-numbered chiral centre being arbitrarily assigned the symbol (*R**). For racemic modifications of compounds containing more than one chiral centre, the symbols (*RS*) and (*SR*) are used, the lowest-numbered chiral centre being arbitrarily assigned the symbol (*RS*).

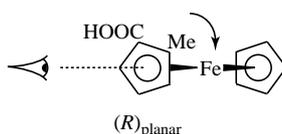
For further information see Cahn, R.S. *et al.*, *J. Chem. Soc.*, 1951, 612; *Experientia*, 1956, **12**, 81; *Angew. Chem., Int. Ed. Engl.*, 1966, **5**, 383; Prelog, V. *et al.*, *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 567.

The use of the (*R,S*)-system for chiral polyhapto complexes is not covered by the original Cahn-Ingold-Prelog rules and further specification of ligand priorities and bonding convention is required.

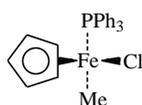
Chiral metallocenes and related complexes. The most widely employed system for specification of metallocene chirality is due to Schögl. The bond from the central metal atom to the ring carbon atom under consideration is treated as a formal single bond. The carbon atom is then considered as a chiral centre and (*R,S*) nomenclature is applied in the usual way.



For further information see Schögl, K., *Topics in Stereochemistry*, 1967, 39. In some older papers, the molecule is considered overall as a case of planar chirality. However, this convention becomes ambiguous when applied to some more complex structures.



Polyhapto ligand as a substituent on a chiral atom. Several conventions have been proposed for determining the order of priority of ligands where one or more is π -bonded. Probably the one most widely accepted is due to Stanley and Baird, in which the ligand is considered a pseudoatom of atomic weight equal to the sum of all of the π -bonded atoms.

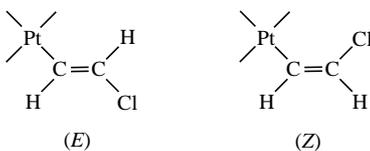


Priority C₅H₅ ('atomic weight' = 60) > Cl > PPh₃ > Me
Chirality (*S*) at Fe

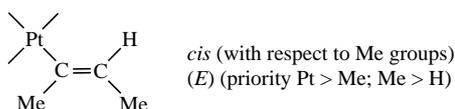
For further information see Stanley, K. *et al.*, *J. Am. Chem. Soc.*, 1975, **97**, 6598.

(b) *The (E,Z)-system*

This is an extension of the (*R,S*)-system for specifying configurations at alkene double bonds. The substituents are ordered as in the (*R,S*)-system and if the two of higher priority are on the same side of the double bond, the configuration is (*Z*) (*zusammen*), while if they are on opposite sides it is (*E*) (*entgegen*).

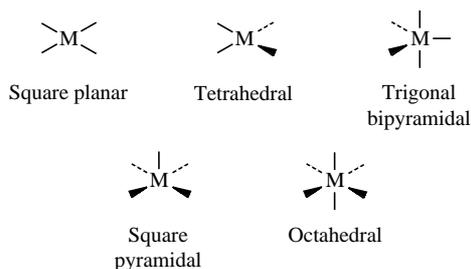


Note that (*E*) does not always correspond to the *trans*- of the earlier literature.



(c) *Coordination polyhedra*

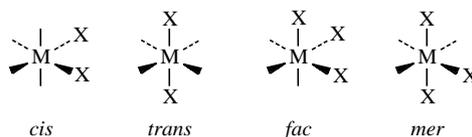
The various coordination polyhedra are depicted using wedged and dashed bonds, the most common polyhedra being:



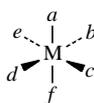
The shapes of polyhedra greater than 6 are not amenable to clear representation by this means and a textual statement such as 'square antiprismatic' is combined with the diagram.

The terms 'tetrahedral' and 'octahedral' are used in a general sense and do not imply strict symmetry types. For the latter, the point group descriptors T_d and O_h are employed.

In the case of **octahedral complexes** bearing two different types of substituents, the stereochemistry is adequately defined using the terms *cis*, *trans*, *fac* or *mer*:



In more complicated cases, italicised letters are used to designate the positions of ligands in various configurations. The letters are assigned thus:

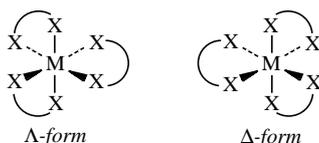


The first mentioned alphabetical ligand in the name is given the designator a , the second ligand the next lowest designator and the assignments to the remaining ligands then follow from this.

Stereochemistry for polydentate ligands is described using the α and β convention:



The absolute configuration of certain octahedral complexes is described using the Δ , Λ convention:



Molecular formula and molecular weight

The elements in the molecular formula are given according to the Hill Convention (C, H and then other elements in alphabetical order). Each entry is assigned a formula. This presents difficulties in the case of incompletely characterised compounds. For such compounds the formula is shown in square brackets to alert the reader to its artificiality. Examples include complexes such as technetium citrate which are important commercially but whose composition has not been determined. Artificial formulae are also used in grouping together series of closely related binary compounds where it is felt their organisation as a family is helpful to readers. For example, tungsten silicides are grouped together in this way. The specific names and formulae for different stoichiometries are all separately presented within the entry and are fully searchable. Molecular formulae of important derivatives are provided.

Molecular weights (or more strictly, molar masses in daltons) given are computer calculated from the formulae using the values for atomic weights of the elements published by the IUPAC Inorganic Chemistry Division, Commission on Atomic Weights and Isotopic Abundances; *Pure Appl. Chem.*, 1991, **63**, 975. Molecular weights are given to one decimal place, but it is important to note that *the atomic weights of some elements are variable within wider limits than this implies*. This applies not only to radioactive or radiogenic elements such as Tc, U or Pb but also to some non-radioactive elements, especially Li and B which exhibit a wider variation in commercially available samples, and Pd which exhibits a wide natural variation.

Source/Synthesis

Brief synthetic details are provided for the majority of compounds, with the aim of apprising the user with the kind of routes available. Formulae are frequently abbreviated to save space (the most common ones are included in Table 1). For full details of conditions necessary to effect transformations, the user is referred to the appropriate literature citations provided. Information about the sources of compounds occurring as minerals or natural products is also given.

Use/Importance

Care has been taken to make the information given on the importance and uses of chemical substances as accurate as possible. Many substances have now been patented for a wide variety of uses, but this does not imply that the patented uses are of widespread applicability or even of established utility. In general, information on the use of an inorganic or organometallic compound is given when it has an established laboratory or industrial application or where it has been shown to undergo or catalyse reactions of potential usefulness. Data in this field may be searched under **Use/Importance** or **All Text**.

Use of organometallic compounds as synthetic reagents is now widespread and this is reflected in the addition of Synthetic Reagents Classification Codes, which are searchable under the **Type of Compound** field.

Physical data

Interatomic dimensions

Selected dimensions, usually obtained by x-ray crystallography, are provided: bond lengths are given in picometres ($\text{pm} = 10^{-12}\text{m} = 10^{-2}\text{\AA}$) and angles in degrees.

Appearance

This data describes whether a compound is solid, liquid or gas and also gives an indication of its colour (even if colourless), crystal form and recrystallisation solvent. Details of air, moisture and thermal stability are also included where available.

Solubilities

Solubilities are quoted either qualitatively, e.g. Sol. THF; or quantitatively, e.g. Sol. H_2O (56g per 100cm^3 at 25°).

Densities and refractive indexes

Densities and refractive indexes are now of less importance for the identification of liquids than has been the case in the past, but they are quoted for common or industrially important substances such as solvents, or where no boiling point can be found in the literature.

Densities and refractive indexes are not quoted where the determination appears to refer to an undefined mixture of stereoisomers.

Melting points and boiling points

These are quoted in degrees Celsius. The policy followed in the case of conflicting melting point data is as follows:

- (a) Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted.
- (b) Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure) the lower figure is given in parentheses, thus: Mp 139° (135–136 $^\circ$).
- (c) Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses, thus: Mp 142° , Mp 205–206 $^\circ$.
- (d) Known cases of polymorphism or double melting point are noted. Many organometallic compounds do not melt sharply due to decomposition at or

below the melting point and to difficulties of complete purification. There are, therefore, numerous examples of wide discrepancies in melting point.

Boiling points are recorded at ambient pressure unless indicated by a subscript representing the pressure in mmHg of the measurement, e.g. Bp₁₀ 140°. Boiling point determination is less precise than that of melting points and conflicting boiling point data is not usually reported except when there appears to be a serious discrepancy between the different authors.

Sublimation points are recorded in a similar style to boiling points, e.g. Subl.₂₀ 150°.

Optical rotations

These are given whenever possible, and normally refer to what the contributor believes to be the best-characterised sample of highest chemical and optical purity. Where available, an indication of the optical purity (op) or enantiomeric excess (ee) of the sample measured now follows the specific rotation value.

Specific rotations are dimensionless numbers and the degree sign which was formerly universal in the literature has been discontinued.

pK_a values

pK_a values are given for both acids and bases. The pK_b of a base can be obtained by subtracting its pK_a from 14.7 (at 20°) or from 14.00 (at 25°).

Spectroscopic data

Spectroscopic data such as ir maxima, uv wavelengths and extinction coefficients are given in many cases where spectroscopic identification has been important in characterisation, particularly for unstable compounds. Efforts have been made, in particular, to include carbonyl and M—H stretching frequencies wherever possible. In many other cases, spectroscopic data can be rapidly located through the references quoted.

Thermodynamic data

Limited thermodynamic data is provided. In many other cases, this information can be located through the references quoted.

Hazard and toxicity information

Hazard and toxicity information is displayed in red type and additionally highlighted by the sign ►.

The field of safety testing is a complex, difficult and rapidly expanding one, and while as much care as possible has been taken to ensure the accuracy of reported data, the *Dictionary* must not be considered a comprehensive source on hazard data. The function of the reported hazard data is to alert the user to possible hazards associated with the use of a particular compound, but the absence of such data cannot be taken as an indication of safety in use, and the publishers cannot be held responsible for any inaccuracies in the reported information.

Many inorganic and organometallic compounds have not been evaluated toxicologically but it is to be assumed that all compounds of certain elements such as As, Be, Hg and Tl are toxic, and that compounds containing certain groups such as perchlorate and azide are likely to be explosive.

The handling of the majority of air-sensitive inorganic and organometallic compounds is to be regarded as hazardous to a greater or lesser degree

because of the risk of fire or explosion in contact with air. Not every such sensitive compound has been specially marked as hazardous. Additionally, many metal halides (often the starting point for organometallic synthesis) can be easily hydrolysed, and all should be regarded as skin, eye and respiratory tract irritants.

*RTECS[®] Accession Numbers**

Many entries in DIOC contain one or more RTECS[®] Accession Numbers. Possession of these numbers allows users to locate toxicity information on relevant substances from the *NIOSH Registry of Toxic Effects of Chemical Substances*. The Registry is a compendium of toxicity data extracted from the scientific literature and each substance is identified by a unique nine-character alphanumeric RTECS[®] Accession Number.

For each Accession Number, the RTECS database provides the following data where available: substance prime name and synonyms; update data; CAS registry number; molecular weight and formula; reproductive, tumorigenic and toxic dose data; citations to aquatic toxicity ratings, IARC reviews, ACGIH Threshold Limit Values, toxicological reviews, existing Federal standards, the NIOSH criteria document program for recommended standards, the NIOSH current intelligence program, the NCI Carcinogenesis Testing Program and the EPA Toxic Substances Control Act inventory. Each data line and citation is referenced to the source from which the information was extracted.

Bibliographic references

The selection of references is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. Thus, in general, recent references are preferred to older ones. The number of references quoted cannot be taken as an indication of the relative importance of a compound.

References are given in date order except for references to spectroscopic library collections, which sort at the top of the list, and those to hazard/toxicity sources which sort at the bottom.

The contents of many references are indicated by means of suffixes. A list of the most common ones is given in Table 2.

Some reference suffixes are now given in **boldface** type, indicating where the editors consider the reference to be particularly important, e.g. the best synthesis giving full experimental details and often claiming a higher yield than previously reported methods.

In some entries, minor items of information, particularly the physical properties of derivatives, may arise from references not cited in the entry.

Journal abbreviations

In general these are uniform with the *Chemical Abstracts Service Source Index* (CASSI) listing except for a short list of very common journals:

DIOC Abbreviation

Acta Cryst.
(and sections thereof)
Angew. Chem., Int. Ed.
Annalen
Chem. Comm.
J.A.C.S.
J.C.S.
(and subsections thereof)
J.O.C.
Tet. Lett.

CASSI

Acta Crystallogr.
(and sections thereof)
Angew. Chem., Int. Ed. Engl.
Justus Liebigs Ann. Chem.
J. Chem. Soc., Chem. Commun.
J. Am. Chem. Soc.
J. Chem. Soc.
(and subsections thereof)
J. Org. Chem.
Tetrahedron Lett.

Table 1. Database abbreviations

Abbreviation	Meaning
[α]	specific rotation
abs. config.	absolute configuration
Ac	acetyl
acac	acetylacetonato
AcOH	acetic acid
Ac ₂ O	acetic anhydride
alk.	alkaline
amorph.	amorphous
anal.	analytical applications, analysis or detection
anhyd.	anhydrous
approx.	approximately
aq.	aqueous
asym.	asymmetrical, unsymmetrical
B	base
BAN	British Approved Name
biol.	bibliography
biol.	biological
biosynth.	biosynthesis
bipy	2,2'-bipyridine
Bp	boiling point
br	broad
BSI	British Standards Institution
Bu	butyl (Bu ^t for <i>tert</i> -butyl etc.)
Bz	benzyl
c.	concentration
ca.	(circa) about
ccp	cubic close packed
cd	circular dichroism
cdt	1,5,9-cyclododecatriene
C ₆ H ₆	benzene
chromatog.	chromatography
C ₅ Me ₅	pentamethylcyclopentadienyl

Abbreviation	Meaning
cmr	carbon (^{13}C) nuclear magnetic resonance spectrum
cod	1,5-cyclooctadiene
compd(s)	compound(s)
conc.	concentrated
config.	configuration
conformn.	conformation
const.	constant
constit.	constituent
coord.	coordinate(d), coordination
corresp.	corresponding
cot	1,3,5,7-cyclooctatetraene
Cp	cyclopentadienyl
C_5Ph_5	pentaphenylcyclopentadienyl
cryst.	crystal(s)
CVD	chemical vapour deposition
Cy	cyclohexyl
d	density
dba	dibenzylideneacetone
dec.	decomposes, decomposition
deg.	degree
degradn.	degradation
depe	1,2-bis(diethylphosphino)ethane
deriv(s).	derivative(s)
descr.	described
detn.	detection, determination
diars	diarsine (generalized ligand)
dil.	dilute, dilution
dimorph.	dimorphic
diphos	generalized diphosphine ligand
diss.	dissolves, dissolved
dissoc.	dissociates
dist.	distil, distillation
DMA	dimethylacetamide
DMF	dimethylformamide
dmpe	1,2-bis(dimethylphosphino)ethane
dmpm	bis(dimethylphosphino)methane
DMSO	dimethyl sulfoxide
dppe	1,2-bis(diphenylphosphino)ethane
dppm	bis(diphenylphosphino)methane
dppp	1,3-bis(diphenylphosphino)propane
dta	differential thermal analysis
ed	electron diffraction
EDTA	ethylenediaminetetraacetate(4-)
ee	enantiomeric excess
E_g	band gap (electron volts)
electrochem.	electrochemistry, electrochemical
em	electron microscopy
en	ethylenediamine
epr	electron paramagnetic (spin) resonance spectrum
equilib.	equilibrium
esp.	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol

Abbreviation	Meaning
EtOH aq.	aqueous ethanol
evapn.	evaporation
exafs	extended X-ray diffraction fine structure
exp.	experimental
fac	facial
Fc	ferrocenyl
fl. p.	flash point
fluor.	fluoresces, fluorescence
formn.	formation
Fp	freezing point
Fp	dicarbonyl(cyclopentadienyl) iron moiety
ΔG°_f	standard free energy of formation
g	gram(s)
glc	gas liquid chromatography
haz.	hazard
ΔH°_f	standard enthalpy of formation
hcp	hexagonal close packed
hplc	high performance liquid chromatography
hydrol.	hydrolyses, hydrolysed, hydrolysis
im	imidazolato
INN	International Non-proprietary Name
inorg.	inorganic
insol.	insoluble
intermed.	intermediate
ir	infrared spectrum
isol.	isolated
isom.	isomerises
J	Joules
JAN	Japanese Accepted Name
K	temperature (Kelvin)
L	generalized ligand
LD	Lethal dose; LD ₅₀ : a dose which is lethal to 50% of the animals tested
lit.	literature
m	medium
M	relative molecular mass (formula weight)
M	metal
manuf.	manufacture(d)
max.	maximum
mcd	magnetic circular dichroism
mCPBA	metachloroperbenzoic acid
Me	methyl
MeOH	methanol
Me ₂ CO	acetone
mer	meridional
mes	mesityl
metab.	metabolism, metabolite
mineral.	mineralogy
misc.	miscellaneous, miscible
mixt.	mixture
MOCVD	metal-organic chemical vapour deposition
mod.	moderately
Mp	melting point
ms	mass spectrum

Abbreviation	Meaning
<i>n</i>	index of refraction e.g. (n_D for 20° and sodium light)
nbd	norbornadiene
nmr	nuclear magnetic resonance spectrum
nqr	nuclear quadrupole resonance spectrum
obt.	obtained
occur.	occurrence
oep	octaethylporphyrinato
OES	occupational exposure standard
O_h	octahedral
op	optical purity
ord	optical rotary dispersion
org.	organic
ox	oxalato
oxidn.	oxidation
pe	photoelectron spectroscopy
Ph	phenyl (C_6H_5)
pH	measure of soln. acidity where $pH = \log_{10}(1/[H^+])$ where $[H^+]$ is the hydrogen ion conc.
pharmacol.	pharmacology
phen	1,10-phenanthroline
photol.	photolysis
phys.	physical
p <i>K</i>	measure of dissoc. const. (<i>K</i>) where $pK = \text{Log}_{10}(1/K)$
pm	picometres (10^{-12} metre)
PMDET	pentamethyldiethylenetriamine
pmr	proton (1H) magnetic resonance spectrum
polarog.	polarography
polym.	polymerised, polymerisation
porph	porphyrinato (generalized ligand)
pptd.	precipitated
pptn.	precipitation
Pr	propyl (Pr^i for isopropyl)
prob.	probably
props.	properties
purifn.	purification
Py	pyridine
pz	pyrazolato
R	generalized alkyl group
redn.	reduction
ref.	reference
rel.	relative(ly)
relat.	related
resoln.	resolution
rev.	review
r.t.	room temperature
S°	standard entropy
s	strong
sepn.	separation
sl.	slightly
sol.	soluble
soln(s)	solution(s)
solv(s)	solvent(s)
soly.	solubility
sp.	species (singular)

Abbreviation	Meaning
spar.	sparingly
spp.	species (plural)
ssp.	subspecies
struct.	structure
subl.	sublimation
synth.	synthesis
tautom.	tautomerism
tbp	trigonal bipyramid(al)
T_d	tetrahedral
temp.	temperature
Tf	triflate
tga	thermogravimetric analysis
thermol.	thermolysis
THF	tetrahydrofuran
tht	tetrahydrothiophene
tlc	thin layer chromatography
TLV	Threshold Limit Value
TMED	tetramethylethylenediamine
tpp	tetraphenylporphyrinato
tox.	toxicity, toxicology
triphos	generalized triphosphine ligand
Ts	tosyl
μ_{eff}	effective magnetic moment (in Bohr magnetons μ_B)
unsatd.	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
uv-vis	ultraviolet and visible spectrum
v.	very
var.	variety
vis.	visible
vol.	volume
Vp	vapour pressure
w	weak
X	generalized anion (usually halide)

Table 2. Reference tags

The following is a selection of the most common reference tags that are used.

Abbreviation	Meaning
abs config	absolute configuration
anal	analysis
bibl	bibliography
biodistribn	biodistribution
biosynth	biosynthesis
cd	circular dichroism
chromatog	chromatography
cmr	carbon (^{13}C) nuclear magnetic resonance spectrum
config	configuration
conformn	conformation
cryst struct	X-ray crystal structure determination

Abbreviation	Meaning
deriv(s)	derivative(s)
detn	detection, determination
dsc	differential scanning calorimetry
dta	differential thermal analysis
ed	electron diffraction
electrochem	electrochemistry, cyclic voltammetry
em	electron microscopy
epr	electron paramagnetic (spin) resonance spectrum
esca	electron spectroscopy for chemical analysis
exafs	extended X-ray diffraction fine structure
fab-ms	fast atom bombardment spectroscopy
glc	gas-liquid chromatography
haz	hazard
hplc	high performance liquid chromatography
ir	infrared spectrum
isol	isolation
isom	isomerism
magnetism	magnetic behaviour/properties
manuf	manufacture
mcd	magnetic circular dichroism
metab	metabolism, metabolite
mineral	mineralogy
Mössbauer	Mössbauer spectrum
ms	mass spectrum
nd	neutron diffraction
nmr	nuclear magnetic resonance spectrum
nqr	nuclear quadrupole resonance spectrum
occur	occurrence
ord	optical rotatory dispersion
pe	photoelectron spectrum
pharmacol	pharmacology
photol	photolysis
pmr	proton (^1H) nuclear magnetic resonance spectrum
polarog	polarography
powder struct	X-ray powder structure determination
props	properties (chemical or physical)
Raman	Raman spectrum
reaction(s)	reaction(s)
resoln	resolution
rev	review
sepn	separation
soly	solubility
struct	structure
synth	synthesis
tautom	tautomerism
tga	thermogravimetric analysis
theory	MO calculations, etc.
thermodyn	thermodynamic data
thermol	thermolysis
tlc	thin layer chromatography
tox	toxicity
trans	transition(s)
use(s)	use(s)
uv	ultraviolet spectrum
uv-vis	ultraviolet visible spectrum