



Science of Synthesis

Houben-Weyl Methods of Molecular Transformations

Information for Authors

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An updated version of “**Information for Authors**” can be found under:
www.science-of-synthesis.com

1 Information for Authors

The publication of **Science of Synthesis** as an electronic version demands absolute consistency of structure and style for the manuscripts. Authors are therefore requested to carefully read and follow the instructions for authors. Furthermore, manuscripts of the appropriate length and style will help to reduce costs and time-consuming editing. This will guarantee the economical and timely publication of **Science of Synthesis**, thus helping to cover the market worldwide. Only manuscripts perfect in style will be suitable for the production of the electronic version of **Science of Synthesis**. Manuscripts which are not written according to these guidelines will not be considered for publication and will be sent back to authors for redrafting. Electronic manuscripts conforming to these guidelines will result in minimum additional work for authors after submission. Authors are strongly encouraged to contact the editorial office (see Section “The People”) concerning all aspects of the manuscripts and to clarify any further questions.

Science of Synthesis is scheduled to be completed in less than 10 years and will then be updated constantly. If a volume is delayed due to pending manuscripts its scientific impact will significantly decrease. We therefore must insist on the timely delivery of manuscripts.

1.1 General Criteria

Science of Synthesis will critically evaluate all existing methods in organic and organometallic chemistry. *The most important molecular transformations for the product class in question must be selected, their scope and limitations should be summarized and they should be illustrated by proven general or typical methods.* Other methods or variations are to be covered in less detail. Further examples for the methods and variations should be summarized in tables. Each method and variation is to be highlighted by a corresponding scheme and an experimental procedure. New aspects of former methods should be extended. The authors should judge the relative merits of different synthetic methods. This should, if possible, result in a ranking of all methods for the product in question. Books, journals, and the patent literature must be considered equally. References to patents should be given whenever they contain relevant information. The authors should not hesitate to contact industrial chemists for procedures reported in patents. For free patent abstracts see www.qpat.com and www.uspto.gov. Care must be taken when evaluating the usefulness of such abstracts since they often give, by necessity, only very general information. Other useful addresses for patent information are www.european-patent-office.org (the European Patent Office), www.wipo.org (Patent Cooperation Treaty, the World Intellectual Property Organization, patent information and patent law), and www.questel.orbit.com (Questel and Orbit search databases and services). IBM's intellectual property resource page (www.patents.ibm.com/respage) provides a useful listing of many patent-related services available online. A useful reference on patent and Markush structure searching is Simmons, E. S., *Drug Discovery Today*, (1998) **3**, 52.

For all methods, references to the pertinent literature must be given. Excessive citation of semirelevant literature should be avoided.

Articles written in the style of monographs or textbooks do not comply with the requirements of **Science of Synthesis**. The manuscript must be written according to the organizational principles as explained in the **Editorial Description** and **Sample Chapter** of **Science of Synthesis**. The sample chapter helps illustrate the editorial style points used and the application of the organizational principles of **Science of Synthesis**. It is requested, at the discretion of the volume editor, that part of the article should be prepared and submitted by the author to the volume editor and the editorial office for approval.

This process will ensure that the individual contribution fits into the general concept of **Science of Synthesis**.

Since **Science of Synthesis** places emphasis on the **synthetic methods of organic chemistry**, mechanism should be discussed if mechanistic aspects are important to explain the occurrence of different products, solvent effects or the stereochemical outcome of a reaction. Authors are encouraged to specifically discuss if a described method has proven to be useful for solid-phase reactions.

1.2 Disposition of the Manuscript

For each volume the editor and the editorial office will specify a general outline which will serve as a guideline to all authors. Authors will be solicited by the volume editor. Authors will then submit for approval to the volume editor a table of contents according to the general outline. *The volume editors and the authors are requested not to exceed the given number of pages for each volume. The authors are asked to contact the volume editor and the editorial office if their manuscripts differ from the agreed length of the manuscript.* For estimating the final length of a contribution, the following general rules should be used (assuming that the author has used the document template):

- 1 typewritten page = 24 lines of 75 characters
- 3 typewritten pages = 1 printed page (without formulas and schemes)
- 2 typewritten pages = 1 printed page (with formulas and schemes)

1.2.1 Organization of the Manuscripts for Science of Synthesis

The authors are requested to follow this general outline for their manuscripts:

1. Author (please give full name, postal address, phone number, fax number and e-mail address).
2. Table of Contents.
3. Text (including tables):
 - Product Class,
 - Product Subclass,
 - Method,
 - Variation.
4. References.
5. Notes to the volume editors or editorial office (comments or additions to the text).
6. Formulas and schemes.
7. Figures (graphs, drawings of apparatus).

The author will write a contribution for a given category and product class and will then organize this manuscript in collaboration with the volume editor and the editorial office into product subclasses, methods, and variations. It is required that authors strictly adhere to the organizational scheme given in the **Editorial Description of Science of Synthesis**. Authors are encouraged to write the introductory texts to the different parts of their manuscripts in the style of a review. These parts should give a general introduction which will help readers to appreciate and understand details of the later-described methods and variations. However, all other parts of the manuscript have a strictly modular organization and should include only information of interest for the given section.

1.3 Guidelines for Text

1.3.1 Format of Texts

Authors must produce their text with word processors. Authors are asked to use the document template (file: scisynth.dot) for their word processors which will be provided by the editorial office (see Section 1.9). Updated versions of the document template can be found under www.science-of-synthesis.com. Additional macros or word processor programming must not be used. The text should be typed with 1.5 times spacing (at least 5 mm between lines) in all parts of the manuscript (including references, notes, figure captions, and tables) and wide margins (ca. 2 cm at top, bottom, left- and right-hand side of each page). We recommend ca. 75 characters per line in a large proportional script (e.g., 12 point Times New Roman). High quality A4 size paper (21.0 × 29.7 cm, 8.3" × 11.6") or US Letter size paper (21.7 × 27.9 cm, 8.5" × 11") should be used. The pages should only be printed on one side. The highest quality for printing should be used. Underlining, indentations, and block capitals should be avoided. Boldface and italic fonts should be used according to the instructions [e.g., amine **6**; *J. Org. Chem.*, (1973) **38**, 3438]. Handwritten additions and underlining, except for volume editors' comments, etc., are to be avoided. References, notes, formulas, schemes, and figures (in this order) should be included at the end of the manuscript. Tables should be included in the appropriate position in the body of the text. All pages including author's address, contents, text, references, notes, and tables must be numbered consecutively. Tables, schemes, formulas, and figures should be numbered with Arabic numbers, not Roman numerals.

1.3.2 Style of the Manuscripts

All parts of **Science of Synthesis** will be written in English. American spelling according to Webster's Dictionary [Merriam-Webster: Springfield MA, (1990)] will be used throughout **Science of Synthesis**. Authors not fluent in idiomatic English are strongly encouraged to ask fluent colleagues for assistance [see also: Schoenfeld, R. *The Chemists English*, VCH: Weinheim, (1990)]. For style of the manuscripts the ACS Style Guide [*The ACS Style Guide*, 2nd ed.; Dodd, J. S., Ed.; American Chemical Society: Washington D.C., (1997)] should be consulted. Authors for **Science of Synthesis** should produce their manuscripts in a style as concise as possible and yet deliver a complete work.

Authors should indicate trademarks and registered trademarks by capitalization of the first letter.

All parts of the manuscript should be written in the **present** or **relevant** tense, except for the **experimental procedures** which should be written in the **past** tense.

1.3.3 Nomenclature

In **Science of Synthesis**, systematic names will be given only to selected examples. "Correct" nomenclature should be used, **based on the rules of IUPAC** [see: *A Guide to IUPAC Nomenclature of Organic Compounds: Recommendations 1993*, Blackwell Scientific: Oxford, (1993)]. Whilst the IUPAC system is preferred whenever possible, names based on the systematic rules adopted by *Chemical Abstracts* (Appendix IV of the current *Chemical Abstracts Index Guide*) will be accepted if necessary, on the understanding that they will in most cases be converted by the editorial office into the appropriate IUPAC-approved form. **Do not use a mixture of both systems**, either within the same name or anywhere within the manuscript. An exception is the naming of ring systems, whose names and numberings may be taken or derived from the *Ring Systems Handbook* [American Chemical Society: Columbus OH, (1988) and supplements]. For biochemical nomenclature see: *Compendium of Biochemical and Related Documents*, Portland Press: London, (1992). Nomenclature

for inorganic compounds is provided by the corresponding IUPAC rules [*Nomenclature of Inorganic Chemistry*, 1970, Butterworths: London, (1971), and *Recommendations*, 1990, Blackwell Scientific: Oxford, (1990)]. In order to facilitate the construction of IUPAC- or CAS-approved names, authors are advised to use a dedicated software program such as ACD/Name (Advanced Chemistry Development Inc., Toronto; http://www.acdlabs.com/products/name_lab/name/), which is utilized by our editorial office. Names of common reagents and solvents are to be retained, e.g. diethyl ether. Trivial names should be avoided unless they offer a distinct advantage over the corresponding systematic name or unless used by prior agreement with the volume editor and the editorial office. For classes of complex natural compounds, such as carbohydrates, peptides, or steroids, the most common name should be given. Compounds which are not named or have long names should be referred to unambiguously as “amine **2**” or “thioester **14**”. In matters of style, i.e. which words or prefixes are hyphenated, italicized, capitalized, etc., consult the ACS Style Guide [*The ACS Style Guide*, 2nd ed.; Dodd, J. S., Ed.; American Chemical Society: Washington D.C., (1997)].

1.3.4 Units

Metric units (SI) should be used throughout the text. However, for pressure and for temperature, Torr/atm/Pa and °C are to be used, respectively [note: 1013.25 mbar = 760 Torr = 101 325 Pa = 14.696 psi]. The unit kcal will also be accepted.

1.3.5 Abbreviations

The use of abbreviations is recommended in tables, formulas, schemes and experimental procedures, but not in titles or text. Common abbreviations used in **Science of Synthesis** are given in the following tables:

Chemical

Name Used in Text	Abbreviation Used in Tables and on Arrow in Schemes	Abbreviation Used in Experimental Procedures
(<i>R</i>)-1-amino-2-(methoxymethyl)pyrrolidine	RAMP	RAMP
(<i>S</i>)-1-amino-2-(methoxymethyl)pyrrolidine	SAMP	SAMP
ammonium cerium(IV) nitrate	CAN	CAN
2,2'-azobisisobutyronitrile	AIBN	AIBN
barbituric acid	BBA	BBA
benzyltriethylammonium bromide	TEBAB	benzyltriethylammonium bromide
benzyltriethylammonium chloride	TEBAC	benzyltriethylammonium chloride
<i>N,O</i> -bis(trimethylsilyl)acetamide	BSA	BSA
9-borabicyclo[3.3.1]nonane	9-BBNH	9-BBNH
borane–methyl sulfide complex	BMS	BMS
<i>N</i> -bromosuccinimide	NBS	NBS
<i>tert</i> -butyldimethylsilyl chloride	TBDMSCI	TBDMSCI
<i>tert</i> -butyl peroxybenzoate	TBPB	<i>tert</i> -butyl peroxybenzoate
10-camphorsulfonic acid	CSA	CSA
chlorosulfonyl isocyanate	CSI	chlorosulfonyl isocyanate

Chemical (cont.)

Name Used in Text	Abbreviation Used in Tables and on Arrow in Schemes	Abbreviation Used in Experimental Procedures
3-chloroperoxybenzoic acid	MCPBA	MCPBA
<i>N</i> -chlorosuccinimide	NCS	NCS
chlorotrimethylsilane	TMSCI	TMSCI
1,4-diazabicyclo[2.2.2]octane	DABCO	DABCO
1,5-diazabicyclo[4.3.0]non-5-ene	DBN	DBN
1,8-diazabicyclo[5.4.0]undec-7-ene	DBU	DBU
dibenzoyl peroxide	DBPO	dibenzoyl peroxide
dibenzylideneacetone	dba	dba
di- <i>tert</i> -butyl azodicarboxylate	DBAD	di- <i>tert</i> -butyl azo-dicarboxylate
2,3-dichloro-5,6-dicyanobenzo-1,4-quinone	DDQ	DDQ
dichloromethyl methyl ether	DCME	DCME
dicyclohexylcarbodiimide	DCC	DCC
<i>N,N</i> -diethylaminosulfur trifluoride	DAST	DAST
diethyl azodicarboxylate	DEAD	DEAD
diethyl tartrate	DET	DET
2,2'-dihydroxy-1,1'-binaphthyllithium aluminum hydride	BINAL-H	BINAL-H
diisobutylaluminum hydride	DIBAL-H	DIBAL-H
diisopropyl tartrate	DIPT	DIPT
1,2-dimethoxyethane	DME	DME
dimethylacetamide	DMA	DMA
dimethyl acetylenedicarboxylate	DMAD	DMAD
2-(dimethylamino)ethanol	Me ₂ N(CH ₂) ₂ OH	2-(dimethylamino)ethanol
4-(dimethylamino)pyridine	DMAP	DMAP
dimethylformamide	DMF	DMF
dimethyl sulfide	DMS	DMS
dimethyl sulfoxide	DMSO	DMSO
di- <i>tert</i> -butyl peroxide	DTBP	DTBP
1,3-dimethyl-3,4,5,6-tetrahydro-pyrimidin-2(1 <i>H</i>)-one	DMPU	DMPU
ethyl diazoacetate	EDA	EDA
ethylenediaminetetraacetic acid	edta	edta
hexamethylphosphoric triamide	HMPA	HMPA
hexamethylphosphorous triamide	HMPT	HMPT
iodomethane	MeI	MeI
<i>N</i> -iodosuccinimide	NIS	NIS
lithium diisopropylamide	LDA	LDA
lithium hexamethyldisilazane	LiHMDS	LiHMDS
lithium isopropylcyclohexylamide	LICA	LICA

Chemical (cont.)

Name Used in Text	Abbreviation Used in Tables and on Arrow in Schemes	Abbreviation Used in Experimental Procedures
lithium 2,2,6,6-tetramethylpiperidide	LTMP	LTMP
lutidine	lut	lut
methylaluminum bis(2,6-di- <i>tert</i> -butyl-4-methylphenoxide)	MAD	MAD
methyl ethyl ketone	MEK	methyl ethyl ketone
methylmaleimide	NMM	NMM
4-methylmorpholine <i>N</i> -oxide	NMO	NMO
1-methylpyrrolidin-2-one	NMP	NMP
methyl vinyl ketone	MVK	methyl vinyl ketone
petroleum ether	PE ^a	petroleum ether
<i>N</i> -phenylmaleimide	NPM	NPM
polyphosphoric acid	PPA	PPA
polyphosphate ester	PPE	polyphosphate ester
potassium hexamethyldisilazanide	KHMDS	KHMDS
pyridine	pyridine ^b	pyridine
pyridinium chlorochromate	PCC	PCC
pyridinium dichromate	PDC	PDC
pyridinium 4-toluenesulfonate	PPTS	PPTS
sodium bis(2-methoxyethoxy)aluminum hydride	Red-Al	Red-Al
tetrabutylammonium bromide	TBAB	TBAB
tetrabutylammonium chloride	TBACl	TBACl
tetrabutylammonium fluoride	TBAF	TBAF
tetrabutylammonium iodide	TBAI	TBAI
tetracyanoethene	TCNE	tetracyanoethene
tetrahydrofuran	THF	THF
tetrahydropyran	THP	THP
2,2,6,6-tetramethylpiperidine	TMP	TMP
trimethylamine <i>N</i> -oxide	TMANO	trimethylamine <i>N</i> -oxide
<i>N,N,N',N'</i> -tetramethylethylenediamine	TMEDA	TMEDA
tosylmethyl isocyanide	TosMIC	TosMIC
triethylbenzylammonium bromide	TEBAB	TEBAB
triethylbenzylammonium chloride	TEBAC	TEBAC
trifluoroacetic acid	TFA	TFA
trifluoroacetic anhydride	TFAA	TFAA
trimethylsilyl cyanide	TMSCN	TMSCN

^a Used to save space; abbreviation must be defined in a footnote.^b py used on arrow in schemes.

Ligands

acetylacetonato	acac
2,2'-bipyridyl	bipy
1,2-bis(dimethylphosphino)ethane	DMPE
2,3-bis(diphenylphosphino)bicyclo[2.2.1]hept-5-ene	NORPHOS
2,2'-bis(diphenylphosphino)-1,1'-binaphthyl	BINAP
1,2-bis(diphenylphosphino)ethane	dppe (not diphos)
1,1'-bis(diphenylphosphino)ferrocene	dppf
bis(diphenylphosphino)methane	dppm
1,3-bis(diphenylphosphino)propane	dppp
1,4-bis(diphenylphosphino)butane	dppb
2,3-bis(diphenylphosphino)butane	Chiraphos
bis(salicylidene)ethylenediamine	salen
cyclooctadiene	cod
cyclooctatetraene	cot
cyclooctatriene	cte
η^5 -cyclopentadienyl	Cp
dibenzylideneacetone	dba
6,6-dimethylcyclohexadienyl	dmch
2,4-dimethylpentadienyl	dmpd
ethylenediaminetetraacetic acid	edta
isopinocampheyl	lpc
2,3-O-isopropylidene-2,3-hydroxy-1,4-bis(diphenylphosphino)butane	Diop
norbornadiene (bicyclo[2.2.1]hepta-2,5-diene)	kbd
η^5 -pentamethylcyclopentadienyl	Cp

Radicals

acetyl	Ac
aryl	Ar
benzotriazol-1-yl	Bt
benzoyl	Bz
benzyl	Bn
benzyloxycarbonyl	Cbz
benzyloxymethyl	BOM
9-borabicyclo[3.3.1]nonyl	9-BBN
<i>tert</i> -butoxycarbonyl	Boc
butyl	Bu
<i>sec</i> -butyl	<i>s</i> -Bu
<i>tert</i> -butyl	<i>t</i> -Bu
<i>tert</i> -butyldimethylsilyl	TBDMS
<i>tert</i> -butyldiphenylsilyl	TBDPS
cyclohexyl	Cy
3,4-dimethoxybenzyl	DMB
ethyl	Et
ferrocenyl	Fc
9-fluorenylmethoxycarbonyl	Fmoc
isobutyl	iBu
mesityl	Mes
mesyl	Ms
4-methoxybenzyl	PMB
(2-methoxyethoxy)methyl	MEM

Radicals (cont.)

methoxymethyl	MOM
methyl	Me
4-nitrobenzyl	PNB
phenyl	Ph
phthaloyl	Phth
phthalimido	NPhth
propyl	Pr
isopropyl	iPr
tetrahydropyranyl	THP
tolyl	Tol
tosyl	Ts
triethylsilyl	TES
triflyl, trifluoromethanesulfonyl	Tf
triisopropylsilyl	TIPS
trimethylsilyl	TMS
2-(trimethylsilyl)ethoxymethyl	SEM
trityl [triphenylmethyl]	Tr

General

absolute	abs
anhydrous	anhyd
aqueous	aq
boiling point	bp
catalyst	no abbreviation
catalytic	cat.
chemical shift	δ
circular dichroism	CD
column chromatography	no abbreviation
concentrated	concd
configuration (in tables)	Config
coupling constant	J
day	d
density	d
decomposed	dec
degrees Celsius	$^{\circ}\text{C}$
diastereomeric ratio	dr
dilute	dil
electron-donating group	EDG
electron-withdrawing group	EWG
electrophile	E
enantiomeric excess	ee
enantiomeric ratio	er
equation	eq
equivalent(s)	equiv
flash-vacuum pyrolysis	FVP
gas chromatography	GC
gas chromatography-mass spectrometry	GC/MS
gas-liquid chromatography	GLC
gram	g
highest occupied molecular orbital	HOMO
high-performance liquid chromatography	HPLC
hour(s)	h

General (cont.)

infrared	IR
in situ	in situ
in vacuo	in vacuo
lethal dosage, e.g. to 50% of animals tested	LD ₅₀
liquid	liq
liter	L
lowest unoccupied molecular orbital	LUMO
mass spectrometry	MS
medium-pressure liquid chromatography	MPLC
melting point	mp
milliliter	mL
millimole(s)	mmol
millimoles per liter	mM
minute(s)	min
mole(s)	mol
nuclear magnetic resonance	NMR
nucleophile	Nu
optical purity	op
phase-transfer catalysis	PTC
proton NMR	¹ H NMR
quantitative	quant
reference (in tables)	Ref
retention factor (for TLC)	R _f
retention time (chromatography)	t _R
room temperature	rt
saturated	sat.
solution	soln
temperature (in tables)	Temp (°C)
thin layer chromatography	TLC
ultraviolet	UV
volume (literature)	Vol.
via	via
vide infra	<i>vide infra</i>
vide supra	<i>vide supra</i>
yield (in tables)	Yield (%)

1.3.6

Experimental Procedures

Experimental procedures should follow the style of the Thieme journal **SYNTHESIS**. The experimental procedure itself is entitled with the product, or general classification of the product name (see example below), and must contain all the information necessary to guarantee reproducibility. This should be followed, where applicable, by the specification of:

- (1) General Procedure: A generalized version of a widely applicable experimental procedure.
- (2) Typical Procedure: A specific example of a widely applicable experimental procedure.
- (3) Single Procedure: Single procedures are not to be labeled but are defined as follows: A specific experimental procedure for a single compound which is not applicable to similar compounds or for which the scope has not been studied.

As the criteria used to assess experimental procedures include range of applicability, the majority of procedures will be Typical or General Procedures; non-typical procedures for individual examples are restricted to unique methods that are particularly useful for the synthesis of one synthetically important compound or intermediate.

The author should indicate aspects of the procedure which are particularly critical to success, including any new observations on or adaptations of older literature methods. Available details of workup should be included. **Authors are encouraged to specifically discuss if a described method has proven to be useful for solid-phase reactions.** Physical or spectroscopic data should be given only to a very limited extent. Authors should choose **significant** spectroscopic data (e.g., shifts of important NMR signals) of the products. These data should help chemists to repeat the procedures and identify the products. The slash symbol is to be used for: (1) surfaces, e.g. Pd/C; (2) alloys and amalgams, e.g. 5% Na/Hg, Na/K (1:1); (3) solvent mixtures, e.g. EtOH/MeOH (95:5); (4) reagent concentrations, e.g. 2% HCl/H₂O; (5) single reagents, e.g. Li/NH₃.

Each procedure title should take the format shown in Section 1.3.6.1 below. This includes the compound number, written in parentheses after the compound name, followed by a colon and then the reference number in superscript square brackets (see Section 1.4). For electronic processing reasons, compound numbers **in procedure titles only** should not be emboldened. Write procedures in the **past** tense and include the weight, number of moles, volume, etc., in brackets **after** the name of the substances or solvents. Avoid starting sentences with numbers, wherever possible.

1.3.6.1 Example of an Experimental Procedure

Tributyl[(R)-1-methoxymethoxy-2-methylpropyl]stannane (4b):^[25]

A soln of crude **3b** (7.3 g, from 15 mmol of **2b**) in THF (40 mL) was cooled in an ice bath and NaOH (1.5 g, 37 mmol) in H₂O (8 mL) was added, followed by dropwise addition of H₂O₂ (30%, 5 mL, 50 mmol). The mixture was kept at 0 °C for 1 h, then at 25 °C for 6 h, during which time a pasty, colorless precipitate formed. The mixture was treated with Et₂O (50 mL) and filtered. The aqueous phase was separated and extracted with Et₂O (3 × 30 mL) and the combined organic phase was dried (MgSO₄) and concentrated. The gel-like residue was flash chromatographed [silica gel, petroleum ether (bp 30–40 °C)/Et₂O 9:1] to give the labile intermediate; yield: 3.98 g (76%); this was reacted further without characterization. To a soln of the intermediate (3.6 g, 10 mmol) in CH₂Cl₂ (10 mL) was added iPr₂NEt (1.2 g, 10 mmol), followed by chloromethoxymethane (0.89 g, 11 mmol). The mixture was stirred for 1 h at 0 °C and 15 h at 25 °C, then concentrated. The resultant residue was treated with ice-cold 2 M HCl (10 mL) and extracted with petroleum ether (bp 30–40 °C, 2 × 20 mL). Concentration of the organic phase (10⁻² mbar) gave the product as a colorless solid; yield: 3.7 g (92%); mp 130 °C.

1.3.7 Safety

Chemicals are associated with two types of hazard: hazards that are a direct result of the physical or reactive properties of a chemical; and hazards posed by the effect of a chemical on biological systems. Flammability and the stability of a chemical in air or towards water may be included in the first group, while the carcinogenic potential of a chemical or its effect on the reproductive system are health hazards due to the biological properties of a chemical. The different hazardous properties that authors should take into consideration when evaluating experimental procedures are as follows:

Physical and reactive chemical hazards:

- Flammability
- Explosive properties

- Stability in air or in contact with water (pyrophoric and water-reactive compounds)
- Incompatibility with commonly-available chemicals and reagents
- Potential for peroxidation
- Oxidizing or reducing properties
- Storage properties

Health effects of chemicals:

- Known human carcinogens and probable human carcinogens according to the International Agency for Research on Cancer (IARC) classifications
- Known human teratogens
- Chemicals known to have an effect on human reproduction
- Chemicals that are irritants to the skin, eyes and respiratory system (data from human exposure or animal tests)
- Chemicals that are corrosive to the skin, eyes and respiratory system (data from human exposure or animal tests)
- Skin sensitizers
- Chemicals that are highly toxic as a result of some specific pharmacological mechanism (e.g., the potent neurotoxin tetrodotoxin)

Hazard information may be found in:

Rhodes, P. H., *The Organic Chemist's Desk Reference*, Chapman & Hall: London, (1995); pp 112–126.

Urban, P. G. (Ed.), *Bretherick's Handbook of Reactive Chemical Hazards*, 6th Edition, Butterworth-Heinemann: Oxford, (1999).

Luxon, S. G. (Ed.), *Hazards in the Chemical Laboratory*, 5th Edition, Royal Society of Chemistry: Cambridge, (1992).

It is important that authors discuss potential hazards of the described compounds. Furthermore, the methods described in **Science of Synthesis** should be discussed in terms of atom economy, as well as their possible impact on the environment. If toxic solvents (e.g., chloroform), toxic catalysts [e.g., mercury(II) chloride], toxic reagents (e.g., phosgene) or any other hazardous compounds are used or recommended in certain experimental procedures, alternatives should be discussed. Safety guidelines should be given for dangerous compounds or procedures. Warnings should be given using the following format:

CAUTION: *Hexamethyltungsten(VI) is known to decompose explosively. Proper safety precautions should be taken during its synthesis, storage, and handling.*

1.3.8 Copyright

It is the responsibility of the author to obtain copyright permission for any figures (see Section 1.7), tables, schemes, or textual information from another source that is to be reproduced in his/her **Science of Synthesis** contribution. Copyright infringement is usually the case when text or figures are taken from books [e.g., Brandsma, L.; Verkruijse, H. D., *Synthesis of Allenes and Cumulenes*, Elsevier: Amsterdam, (1981)] or serial publications [e.g., *Organic Synthesis, Coll. Vol. VI*, Noland, W. E., Ed; Wiley: New York, (1988)] without significant adaptation of the original version. In the case of reproduction of experimental procedures and schemes from journal publications a full citation in the references section is sufficient acknowledgement of copyright ownership. The copy editor assigned to each manuscript will ask the author to apply for copyright if they have not already done so, and will add the appropriate credit line. If there is an appropriate and adequate alternative to a reference requiring copyright then this reference should be substituted, or if a similar procedure is available then this procedure should be used instead of that under

copyright. If the author cannot obtain permission then the text will be deleted. Permission request forms are in the author's information package or can be obtained from the editorial office. The editorial office will help authors to direct their applications to the appropriate departments.

1.4 Guidelines for References

References should be placed collectively at the end of the text (in Part 4 of your manuscript, entitled "References") and numbered consecutively within chapters, with no subdivisions such as ^[3a], ^[3b], ^[3c], etc. *Each reference number should contain only one citation.* Use one reference number for each reference only, do not repeat a reference citation with a new number every time it appears. References to literature appear in the text, tables, and scheme headings as superscript 10 pt Arabic numerals in square brackets following the punctuation, e.g. This is a sample sentence.^[1] Authors should include reference numbers for schemes and figures in the scheme/figure caption; reference numbers for tables should be included in the tables as the final column. To facilitate the production of the electronic version of **Science of Synthesis**, the references do not follow the rules as given in the ACS Style Guide [*The ACS Style Guide, 2nd ed.*; Dodd, J. S., Ed.; American Chemical Society: Washington D.C., (1997)]. Authors are requested to ensure the accuracy of the references.

Journals: provide the names of **all** authors. Do not use "et al.". A comma should be used to separate the name of the last author and the title of the journal. Use the journal abbreviation in accordance with *Chemical Abstracts* [*Chemical Abstracts Service Source Index (CASSI) 1907–1994 Cumulative* and its supplements].

Science of Synthesis will support the citation of electronic journals. As soon as general document identifiers for journal articles are available, the editorial office will include them to allow users direct access to these references.

Books: see sample references for books with and without editors.

Patents: see sample reference. Important patents should be read in the original versions as *Chemical Abstracts* reports often do not contain all important details.

Databases: reference can also be given to records in databases (e.g., spectra from databases like Specinfo).

If reference is made to a patent or less readily available journal, the *Chemical Abstracts* reference or the English translation [e.g., *J. Gen. Chem. USSR (Engl. Transl.)*] should also be cited.

The use of a reference-managing program (e.g., EndNote) is strongly recommended.

1.4.1 Sample References

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1.5 Guidelines for Tables and Scheme Tables

Tables should be used to display examples of similar products prepared by a given method or variation in order that they may be critically discussed in the text. **Do not list every example known; only selected examples should be given.** Tables should contain 5 to 10 examples and should be placed in the appropriate position in the body of the text. Tables should be numbered with Arabic numerals and have captions with initial letters of major words capitalized. When referring for the first time to information given in a table, please quote the table number in brackets. The position of a table should be indicated in the text in the following way:

< **Table 1** > This is a Sample Caption

In tables, collect comparable examples and quote, in the following order:

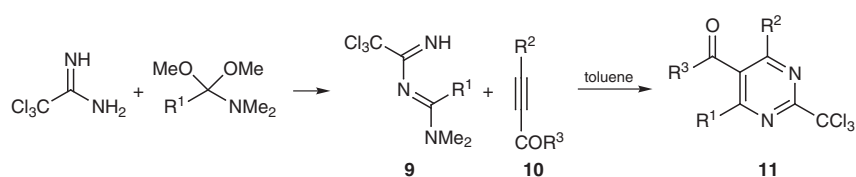
- (1) The starting material represented pictorially, e.g. either present a generalized equation above and then give only substituents R¹, R², X, etc. (*vide infra*) or, in the case of structurally diverse substrates, give the entire formula. An entry number is also acceptable for identifying the starting material. In all cases, arrange the examples in a manner which best illustrates the scope and limitations of the method (e.g., they may be listed in increasing order of substituent/reagent complexity, or in increasing order of chemical or optical yield, etc.).
- (2) Reagents, solvents, temperature, times, as applicable.
- (3) Product (formula or entry number).
- (4) ee, er (preferred), dr when applicable.
- (5) Yield data.
- (6) Physical data, if relevant (e.g., mp).
- (7) Citation of the relevant literature.

< **Table 1** > Caption

Starting Material	Reaction Conditions I	Reaction Conditions II	Product	er or dr	Yield (%)	Ref
(formula or entry number)	(reagents, catalysts, solvents)	[Temp (°C), pressure (mbar)]	(formula or entry number)			

Scheme tables should be employed in conjunction with schemes if the latter are likely to become over-cluttered with textual notes. They should be used to illustrate methods (or variations) when: (1) there are 8 or more examples for the method but they are not actively and individually discussed in the main text, and thus presented in a normal table (*vide supra*); (2) there are fewer examples but they contain several varying R-substituents on the reagent(s) in the scheme; (3) there are different conditions (e.g., solvent, temperature, ratio of reactants) employed for the same reaction which have a significant influence on the yield, purity, or optical purity, etc. of the product. All other cases should simply include the examples within the scheme itself (*vide infra*).

The content and layout of a scheme table should be similar to that employed for a table, and in all cases kept as simple as possible. An example of a scheme table is given below:



R ¹	R ²	R ³	Ratio (9/10)	Conditions	Chromatography Eluent, Ratio (hexane/EtOAc)	Yield (%)	Ref
H	CO ₂ Me	OMe	1:4	rt, 30 min	4:1	98	[21]
H	H	OEt	1:4	70 °C, 24 h	4:1	75	[21]
H	Ph	OMe	1:2	101 °C, 30 h	9:1	51	[21]
H	H	H	1:1	rt, 30 min	85:15	66	[21–23]
Me	CO ₂ Me	OMe	1:4	rt, 30 min	9:1	76	[21–23]
Me	H	OEt	1:4	80 °C, 1 h	9:1	65	[21, 22, 36]
Ph	CO ₂ Me	OMe	1:4	rt, 30 min	85:15	73	[36]
Ph	H	OEt	1:4	80 °C, 3 h	9:1	56	[36]
Ph	Ph	OMe	1:2.7	101 °C, 4 h	9:1	40	[36]
Ph	H	H	1:1.3	rt, 1 h	9:1	43	[23, 36, 45]

Scheme tables should be placed below the relevant scheme heading in the body of the text. Scheme tables will not have a caption but **<Schemetable n>** should be used as a pointer in the main text.

1.6 Guidelines for Formulas and Schemes

The formulas and schemes should be visual abstracts of the reactions performed, hence flow diagrams are preferred to individual structures.

Formulas and schemes should be numbered with Arabic numerals and have captions with initial letters of major words capitalized. When referring for the first time to information given in a scheme, please quote the scheme number in brackets. Captions will not be listed at the end of the manuscript and will instead stay in the manuscript. A formula or scheme should be indicated in the text in the following way:

<Formula 1> This is a Sample Formula

<Scheme 1> This is a Sample Scheme

Formulas and schemes should be placed separately in Part 6 of your manuscript. Formulas, schemes and figures must be submitted on a separate sheet. They should **not** be electronically embedded in the text.

Formulas and schemes should not exceed a width of 16 cm; schemes wider than this will not be accepted. Bonds and reaction arrows should be placed vertically, horizontally or at 45° angles. Authors should try to make economic use of the space. Products (and substrates and intermediates that are referred to in the text) should be numbered with bold,

Arabic numbers from left to right in sequence as they appear in the schemes. Begin from **1** at the start of each product class. Every compound in a scheme does not have to have a number. If a compound is mentioned in the text it must have a number and the title compound in an experimental procedure should also have a number. For compounds with different substituents, the labels R¹, R², X, etc. must be used and explained below the reaction scheme or in a table. Do not use R without a superscript. Use ⁺ and ⁻ (i.e., plus and minus symbols as superscripts) for electric charges (do not circle them). Two dots should be used to indicate a lone pair. Do not summarize several reaction steps by using only one reaction arrow. Each reaction arrow should symbolize only **one** single reaction. Reagents, conditions, etc., should appear above the arrow. Unstable intermediates should be drawn in square brackets (see below). Each individual reagent, condition, etc., should be separated from the next by a comma and one character space, not a semicolon or slash; no comma should appear at the end of a line. Reagents, conditions, etc., appear in the following order:

- (1) Reagents, including catalysts, e.g. H₂(g), Pd/C, (Ph₃P)₄Pd.
- (2) No. of equivalents.
- (3) Solvents.
- (4) Special apparatus, e.g. sealed tube, autoclave.
- (5) Temperature, e.g. rt, 50 °C, reflux.
- (6) Pressure, e.g. 20 mbar, 100 Pa.
- (7) Time, e.g. 5 min, 12 d, 6 h.

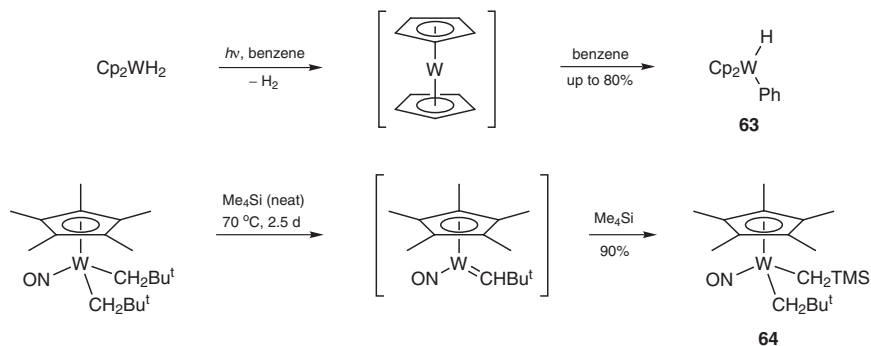
Eliminated products (preceded by a minus sign) and the reaction yield appear below the arrow. References will not appear in schemes but in the scheme headings.

For intermediates in schemes the following rules apply:

1. Isolable intermediates are to be included in schemes and will get put into a separate reaction database for reaction searching.
2. Elusive intermediates and transition states can also be put into schemes but they will not be included in the reaction database. They should be placed within square brackets.

Scheme 1 shows an illustrative example of a reaction scheme.

Scheme 1 By Oxidative Addition of Alkanes and Arenes^[108, 110]



For drawings prepared by CSC ChemDraw, use the following settings, printed at 100% (page setup = 100%). Authors using different drawing programs are requested to use settings which are consistent with those below. Please do not use wedged bonds (bold or hashed) to represent chiral centers; use normal bold or hashed bonds instead (see Sample Chapter).

Choose settings type:	Science of Synthesis, except for the margin width	
Font for atoms, reaction conditions, yield and captions:	10 point Helvetica or Arial	
Chain angle:	120 degrees	
Bond spacing:	18% of length	
Fixed length:	17 point	(0.600 cm, 0.236")
Bond width:	2.0 point	(0.071 cm, 0.027")
Line width:	0.8 point	(0.028 cm, 0.011")
Margin width:	2.2 point	(0.079 cm, 0.031")
Hash spacing:	2.5 point	(0.088 cm, 0.035")

1.7 Guidelines for Figures

Figures should be numbered with Arabic numerals. When referring for the first time to information given in a figure, please quote the figure number in brackets. Figure captions will not be listed at the end of the manuscript and will instead stay in the manuscript. A figure should be indicated in the text in the following way:

< **Figure 1** > This is a Sample Figure

Figures should be placed separately in Part 7 of your manuscript. Figures must be submitted on a separate sheet. They must **not** be electronically embedded in the text.

If necessary, figures will be redrawn by the publishers. For checking and correction, the redrawn figures will be sent back to the author. In the case of figures taken from existing publications, **it is the legal responsibility of the author to obtain permission for reproduction from the copyright holder**; this should be done at a very early stage of the book production. For figures of apparatus, please directly contact the apparatus producer company. If figures are not produced by the author, the copyright of the figure must be included in the caption. Submit only original figures or high quality photographic prints of originals. For the preparation of graphs, authors are requested to follow the suggestions of H. G. Hers [*Nature*, (1984) **307**, 205]. The highest resolution of the printer available should be used for the printouts.

1.8 Delivery of the Manuscripts

Authors are requested to send one copy of their table of contents to the editorial office and one copy to the appropriate volume editor. Authors will then receive a revised table of contents with comments and suggestions from both the volume editor and the editorial office.

Authors are requested, after approval of their table of contents, to submit a four-page sample of their work. This document should be a short example of the type of format the author envisages their final manuscript being submitted in. Sample pages should contain, where appropriate, examples of:

- Introductory text,
- Experimental procedures,
- Tables,
- Schemes,
- Figures,
- References.

The sample pages should also have the document template styles applied to them wherever possible. Sample pages should be submitted on disk as detailed under Section 1.9 with a printout corresponding exactly to what appears on the disk. Submission of these sample pages enables the in-house copy editors to give feedback on editorial issues. It also

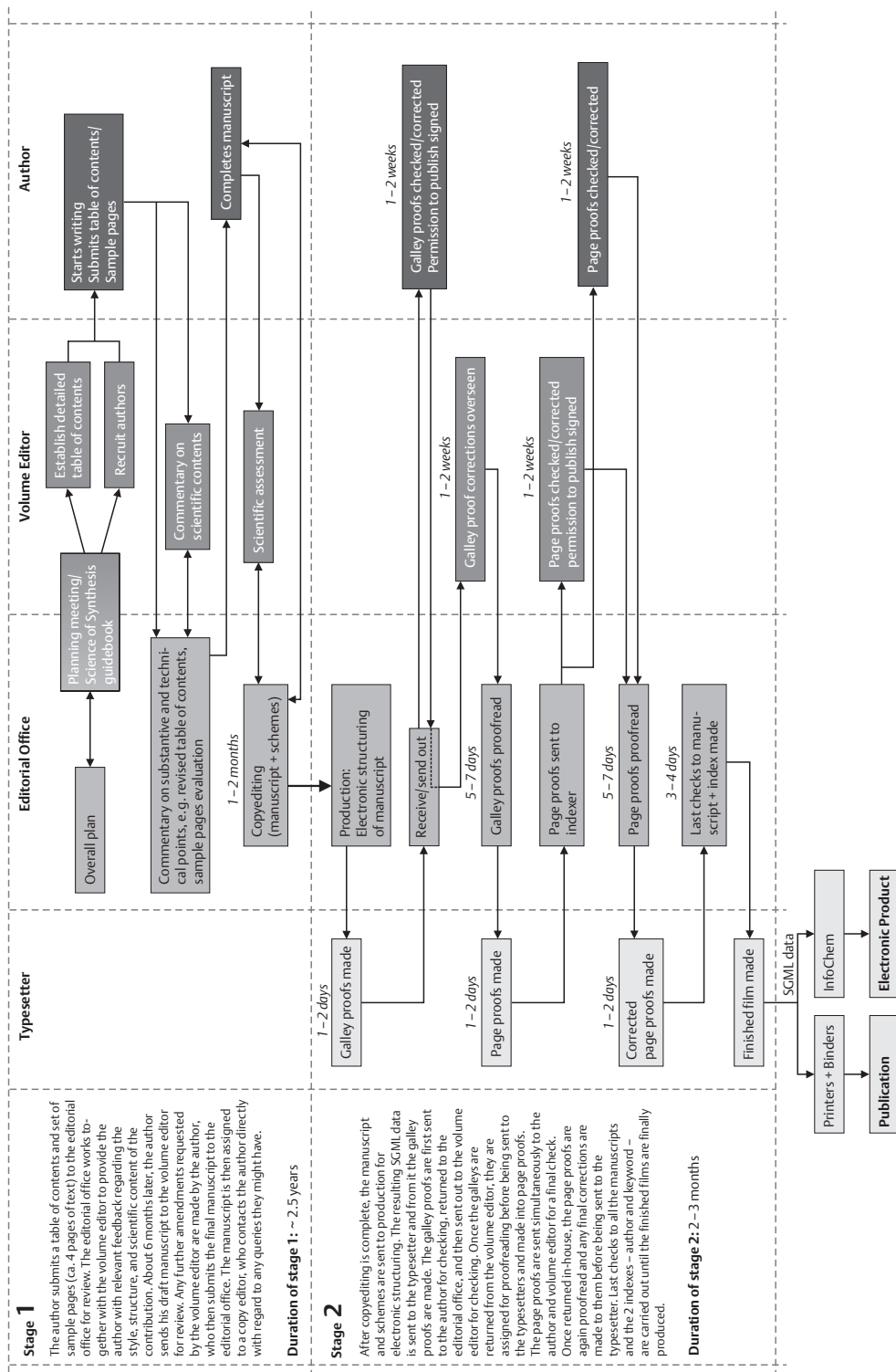
enables the author to identify potentially problematic issues regarding their manuscript. Sample chapter evaluations will be provided to authors after final approval from the appropriate volume editor. It is possible to see an example of how we would like a **final manuscript** to be presented by downloading the document template files from the **Science of Synthesis** website and looking at the file **elecsamp.doc**. If there are any questions regarding sample pages do not hesitate to contact the editorial office.

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The manuscript submitted to the editorial office will then be assigned to a copy editor who will copyedit the manuscript and apply the necessary styles for **Science of Synthesis**, e.g. check nomenclature, grammar, syntax, punctuation, phrasing, redundancy of text, and the like. Copy editors will correspond directly with authors regarding any queries and try to resolve them before proceeding to the galley proof stage. It is inevitable that corrections will still need to be made to the galley proofs, but each copy editor will aim to eliminate as many errors as possible prior to this stage by editing the manuscript thoroughly. The editorial office will then use the manuscripts for the production of the electronic version and prepare them for typesetting. At this stage galley proofs will be sent to the author for correction. The correction of galley proofs should be limited to the correction of printing errors or other mistakes and should not involve major changes to the text. If more extensive corrections are necessary as a result of significant new developments, the volume editor should be consulted. The author may be required to provide additional information at the galley proof stage, in order to comply with the above instructions. Please note that the symbols ■■■ indicate that something was missing or unclear in the manuscript and the pertinent information should be added during correction. The galley proofs should be returned to the editorial office by the deadline given. The author's responsibilities end with the correction of the galley proofs. The author then signs the galley proofs as a permission to publish the manuscript (*Imprimatur*). By accepting a manuscript the publisher acquires all rights, in particular copyright and the right of translation.

The page layout of the contribution follows the proof correction, i.e. the text is laid out to the exact page length, the pages are numbered, tables, formulas, schemes and figures are placed as near as possible to the positions indicated by the author in the galley proofs. Page proofs will subsequently be sent to the volume editor and the author. It is requested that corrections in the page proofs be limited to the elimination of printing errors. The proof sheets are not indicative of the quality of the final print.

Workflow Chart for Science of Synthesis



1.9 Guidelines for the Preparation of the Manuscripts on Disks

In general, the editorial office can process disks in either DOS or Macintosh format. The following word-processing programs are preferred: MS Word 5.0, Word for Windows 2.0 and 6.0, MS Word 97, MS Word 2000, Word Perfect 8 (for PCs) and MS Word 5.1a, 6.0.1, 98, Word Perfect 3.5 (for Mac). The authors will be provided with style templates for these programs. The use of LATEX and DTP programs should be avoided. The **Science of Synthesis** template document contains a list of formatting styles that have to be applied to the chapter captions of your manuscript. The file is called **scisynth.dot**. However, the manuscript will not have the same print format as shown in the sample chapter. The sample chapter as it appears by using the template can also be found on the same disk **elec-samp.doc**. This file is intended to illustrate how the template should be used. It also shows that at this stage manuscripts do **not** have the same format as in print.

Label the disk with the product class, the name of the author(s), the date, the platform, and the version of software used. Check disks with a virus-checking program before submission. Disks containing viruses will not be processed at the editorial office. The electronic version must **exactly** match the hardcopy version. Authors are strongly encouraged to check vigorously the final version for correct spelling and consistency of structure and style.

Author's address, contents, text including tables, references, and notes should be, in this order, in one file. Schemes, formulas, and figures have to be supplied in separate files on disk. Use the formula, scheme or figure number as the file name, e.g. FIGURE1.TIF. The filename of the corresponding formula, figure, or scheme on the accompanying disk should be included (handwritten) at the place where it appears in the text (below the caption):

< **Figure 1** > This is a Sample Caption
handwritten addition: *figure1.tif*

Authors should use only predefined formats and linefeeds to mark paragraphs and document sections. Additional formatting information like separating lines should be omitted. End-of-line hyphenation should be turned off and the text should be left-justified. Do not insert spaces before punctuation. **“Carriage return” should only be used to mark the end of a paragraph, title or heading.** Only one font type should be used (e.g., 12 point Times New Roman) throughout the text. Special characters such as Greek symbols must not be presented as graphical objects. Use the “Symbol” font set and present them as normal characters. Files should be saved in the normal document format of the word-processing program, instead of as plain ASCII text files. RTF files are also acceptable.

Tables should be prepared in the word-processing programs by using tabulators or the automatic table setup instead of space bars. Tables generated in the Microsoft Excel worksheet format are also acceptable.

Formulas and schemes are most preferably generated by ChemDraw (latest version, both for Microsoft Windows or Macintosh) or by ISIS/Draw (MDL Information Systems, Inc., San Leandro, CA; latest version available at: www.mdli.com). They should be saved both in the usual ChemDraw or ISIS format **and** MDL Molfile format (this format is supported by nearly all structure-drawing programs). Reaction centers (the atoms of the molecule which actually participate in the reaction) should be marked in the hardcopy (see Section 1.6).

Figures should be stored in one of the following formats: TIFF (preferred bitmap format), CDR (CorelDraw), HPGL (preferred vectorgraphic format), PostScript (PS), or Encapsulated PostScript (EPS).