UNIVERSITY OF CAMBRIDGE | Yusuf Hamied Department of Chemistry

Successful Completion of a Research Degree: Guidelines for Experimentalists

2023-24

Deborah Longbottom & David Morgan

Table of Contents

1.0 General Information

1.1 General Experimental

This will vary depending on which group you are in and the nature of your project so it is sensible to use a recent (potentially related) thesis to help you get it right. Take care not to just assume that this is correct for your case however:

- Do not just copy your general experimental from a previous thesis: always check that the information is up to date (including the details of the instruments used).

- Make sure you include all information for each type of data gathered plus the instrument used, as given in this document or recommended by your group.

1.2 Naming compounds

It is best to name your compounds according to the IUPAC convention.

https://iupac.org/what-we-do/nomenclature/brief-guides/

If you use ChemDraw to name your compounds, always check the name to ensure it fits with the IUPAC recommendations.

1.3 Numbering compounds

Use the numbers from the IUPAC name to number the compound structure in your experimental section and those numbers in assignment of the data. If you do not for some reason, e.g. you use final natural product numbering on intermediates, make this clear underneath the picture of the compound.

1.4 Characterisation

When characterising compounds, it is important to have in mind that you are able to prove both the *identity* and *purity* of your compounds. Many commonly used techniques focus on identity but do not necessarily assess purity.

Although the specific type of characterisation required might vary depending on what kind of compounds you are making, e.g. organic small molecules may have different requirements to air sensitive inorganic compounds, characterisation is always very important because if you do not have the right evidence to prove you have made what you claim to have made, the results and discussion are not substantiated. Without this solid basis on which to build the R&D section, nothing can be written with certainty.

2.0 Data for Known and Novel Compounds

This depends on whether the compound is known or novel and your supervisor may take a definite view on what should always be included so *always check the group policy in case you are routinely required to do more than is outlined here*. Generally, if you are making **organic molecules** e.g. in a methodology or total synthesis project, the table below gives an outline of the basic minimum requirements:

Criteria	**Known Compound**	**Novel Compound**
Minimum pieces of data:	1 (2 if mp in addition)	4 (5 if mp in addition)
Data which should always be included:[1]	**^{1}H** (oils/liquids) *or* **^{1}H & melting point** (crystalline solids). Cite literature data (usually at end of compound name) and state that all data were identical.	**^{1}H, ^{13}C, IR, HRMS, melting point** (crystalline solids)
Data often included *in addition to* the minimum:[1]	**^{13}C NMR, TLC** (R_F, solvent), **IR**, **LRMS**.	**TLC** (R_F, solvent), **UV/vis**, **other NMR** e.g. P, B, F.
Data which can (known)/should (novel) be included if compound is chiral:	**ee or er** (when excess of one enantiomer over the other) as determined by chiral HPLC / LC / SFC / GC etc. **$[\alpha]_D$** required in addition (whatever the (non-zero) ee is), i.e. both pieces of information needed together. In a methodology project, use the best ee for the $[\alpha]_D$, i.e. no need to get the $[\alpha]_D$ for each product formed during the optimisation process.	
Other information which should be included:	When **flash column chromatography** is used for product purification, both the support (e.g. silica/alumina) & solvent should be identified; **colour and state of the product** should be routinely given, e.g. green amorphous solid, pale pink oil. Crystal shape should be described, e.g. needles (1D), plates (2D) or blocks (3D). More detailed shape description may be possible with a crystal structure.	
What else?	Always **reference the paper** used to compare the data with.	**Elemental analysis** can be used to show purity; **X-ray** structure.

If you are making **air sensitive inorganic compounds**, the requirements alter. Most often, a *crystal structure* will be the single most important piece of data that needs to be obtained. After that, *NMR* is often looked at closely (but may be proton with another element e.g. boron, i.e. less need for ^{13}C), as well as *elemental analysis. Mass spectrometry* is much rarer and *IR*, *melting point* and *TLC* are used very infrequently, if at all.

[1]You need to check with your PI as to the group policy on this: some groups will insist on both ^{1}H *and* ^{13}C NMR *always* being included for a *known* compound, as well as a *novel* one (in line with high profile journals) but for others, ^{1}H alone (oils/liquids) will be the basic requirement. For crystalline solids, ^{1}H and mp should be routinely included, i.e. mp is not usually seen as optional data.

3.0 Level of Detail to Include

In the table below are the Departmental guidelines (see **5.0** for examples) but *always check with your supervisor as to the specific policy of your group before you start* in order that you are adhering to what is expected by your PI.

Technique	Level of Detail
NMR (^{1}H to 2 dp; ^{13}C to 1 dp, unless signals very close: then quote 2 dp or put '2C' in brackets after the number; *J* to the nearest 0.5 Hz)[2]	**Known organic compound**: Although it is essential that you can assign your compounds with confidence, for known compounds, it is not essential to write out the assignment of all peaks in your experimental section. Showing that they match literature data is the important thing. **Novel organic compound**: It is essential that you can assign all novel compounds with confidence in order that you are certain of what you have made. This may not require 2-D data if the compounds are not complicated but, if you cannot assign all the peaks without it, it is wise to have all the 2-D data on at least key intermediates and late stage novel compounds for certainty of what you have made and putting those assignments into the experimental section. **Air sensitive inorganic compound:** ^{1}H and ^{13}C may be useful, as well as other elements, e.g. boron. Occasionally, compounds are paramagnetic and NMR peaks may be too broad to be useful, making crystal structure even more crucial.
IR	Report all major peaks, describe shape e.g. br, weak, strong and assign those which correspond to the functional groups present in your product (for **known and novel organic,** often not required for **air sensitive inorganic**)
MS	**Known organic compound:** LRMS sufficient (LCMS included) **Novel organic compound:** HRMS required within ±5 ppm of calculated value. **Air sensitive inorganic:** often not required.
Melting point	Useful piece of data for both **known organic** (compare with literature value) and **novel organic** (provides comparison for future syntheses) crystalline solid compounds. Always give the range. Often put in brackets the last solvent a compound has been dissolved in. Less useful for amorphous solids as they often melt over a broad temperature range. Often not required for **air sensitive inorganic** compounds.
Elemental analysis	Available in the Department. Supports *purity* of product (cannot see inorganic salts by NMR, IR, MS etc). Not usually needed for **known** compounds. *Unambiguous purity determination (*H% quoted to nearest 0.05%, all other elements to nearest 0.1%) for **novel organic** (within ±0.4% absolute of predicted value) and **air sensitive inorganic** (usually to ±0.5% of predicted). For C, H, N analysis, 1.5 mg minimum for submission, 5 mg plenty. More may be required if elements other than CHN are being analysed.
$[\alpha]_D^{24}$	A non-zero value supports compound being a non-racemic substance. Temperature, solvent and concentration are also stated.
TLC [3] (R_F, solvent)	If you use TLC to help you in making a compound, (unless the compound will not move on the plate) quote this data for **known & novel organic** compounds: it's easy and useful in addition to other data. Not usually required for **inorganic** compounds
X-ray structure	For both **organic & inorganic** compounds, the CCDC number is useful but not essential. Otherwise, you need to include the cif file. For **air sensitive inorganic** compounds, the crystal structure is the most important piece of data.
UV/Vis	If your molecules contain a chromophore that can be monitored or characterized by UV/Vis spectroscopy, then at the very least you should report the wavelength of the recorded absorptions. For pure compounds, reporting the extinction coefficient (ε) provides important information about the properties of chromophore.

[2]Check with your supervisor: for some groups, 1 dp will be the agreed accuracy (see example exp data) but it can be argued that quoting *J* values to the nearest 0.5 Hz better reflects the actual resolution of the spectrometer.

[3]When following a published preparation or previous thesis, this is often the most useful piece of information when you are at the bench.

4.0 Other Potential Situations and the Data to Include

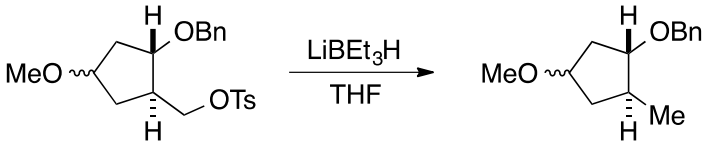
Below are the Departmental guidelines but always check with your supervisor as to the specific policy of your group before you start in order that you are adhering to what is expected by your PI.

Situation	Data to Include
Unpurified compound taken forward to next step crude.	^{1}H NMR data at minimum should be included. The next compound in the synthetic sequence which is purified should then be fully characterised (if **novel**) or match with the available literature data (if **known**). Mass returned from the experiment may be quoted but yield should not. Yields should only be quoted for materials of demonstrated purity.
Compound made previously in the group but synthesis not yet published, e.g. thesis submitted or publication awaiting acceptance.	If the compound has been *fully characterised* previously and the source can be referred to (in enough detail that somebody repeating the procedure can locate it) it can be treated as a **known** compound. If it has *not been fully characterised* in the source, the compound should be treated as **novel** and fully characterised.
Known compound made by a new route.	Treat as a known compound for data comparison purposes. Consider whether the data you have obtained properly proves the purity of the compound made by your method.

5.0 Examples of Experimental Write Up

5.1 Example of How to Write Up the Experimental for a Known Compound (ACS Settings)[4]

Methyl 3-O-benzyl-2,5-dideoxy-D-ribofuranoside (**9**)



8 **9**

To a solution of tosylate **8** (8.74 g, 22.3 mmol) in THF (44 mL) was added $LiBHEt_3$ (44.6 mL of a 1 M solution in THF, 44.6 mmol) at room temperature, and the reaction mixture was stirred at room temperature for 15 min and then at 45 °C for 6 h. The reaction mixture was cooled to 0 °C, and 3 M NaOH solution (5 mL) and 30% H_2O_2 (10 mL) were carefully added. After evolution of hydrogen had ceased, the reaction mixture was concentrated to half of the volume under reduced pressure and extracted with EtOAc. The extract was washed with water (30 mL) and brine (30 mL), dried and concentrated under reduced pressure. Purification by flash column chromatography (20% EtOAc in hexane) afforded **9** (4.56 g, 92%, 50:50 mixture of diastereomers by ^{1}H NMR) as a colorless oil.

$[\alpha]_D^{24}$ +54.3 (*c* 1.40, $CHCl_3$); IR ($CHCl_3$) 1496, 1454, 1365, 1097, 1049, 987 cm^{-1}; ^{1}H NMR (400 MHz, $CHCl_3$) δ 7.34-7.26 (5H, m), 5.06 (0.5H, dd, *J* = 5.4, 1.5 Hz), 4.98 (0.5H, dd, *J* = 5.9, 2.0 Hz), 4.57 (0.5H, d, *J* = 12.2 Hz), 4.49 (0.5H, d, *J* = 12.2 Hz), 4.50 (1H, s), 4.20–4.09 (1H, m), 3.95 (0.5H, ddd, *J* = 6.3, 6.3, 3.9 Hz), 3.62 (0.5H, ddd, *J* = 9.8, 5.4, 3.9 Hz), 3.38 (1.5H, s), 3.34 (1.5H, s), 2.32 (0.5H, ddd, *J* = 13.7, 8.3, 5.9 Hz), 2.24 (0.5H, ddd, *J* = 13.7, 6.4, 2.0 Hz), 2.11 (0.5H, ddd, *J* = 13.7, 5.4, 5.4 Hz), 1.96 (0.5H, ddd, *J* = 13.7, 3.9, 1.4

[4]Taken from the SI for T. Sakai, H. Asano, K. Furukawa, R. Oshima and Y. Mori, *Org. Lett.,* ASAP, April 9th 2014.

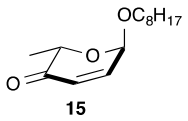
Hz), 1.31 (1.5H, d, *J* = 6.8 Hz), 1.25 (1.5H, d, *J* = 6.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 138.0, 128.4, 128.37, 127.7(X2), 127.64, 127.61, 105.1, 104.3, 83.6, 83.1, 80.0, 77.8, 71.7, 71.67, 54.9, 54.8, 39.3, 38.9, 21.2, 18.9. Spectroscopic data were identical with those reported in the literature (Ye, S.; Rezende, M. M.; Deng, W.-P.; Herbert, B.; Daly, J. W.; Johnson, R. A.; Kirk, K. L. *J. Med. Chem.* **2004**, *47*, 1207–1213).

Notes:

- The authors have given more data than is suggested as part of the notes earlier on. Follow these notes and your group guidelines on the number of pieces of data needed for a known compound.
- The ^{1}H NMR data presented here is a good example of where spectrometer lack of resolution gives different coupling constants: the second signal 5.06 (0.5H, dd, *J* = 5.4, 1.5 Hz) is coupled to 1.96 (0.5H, ddd, *J* = 13.7, 3.9, 1.4 Hz) and the 1.5 and 1.4 Hz couplings should be the same. This is a rounding error associated with the resolution.
- You do not necessarily need to draw the reaction scheme as they do here. It is fine to just draw the compound that has been made if that is your preference.
- You can choose which kind of text setting you like for the main body of text.

5.2 Example of a How to Write Up the Data for a Novel Compound (RSC settings)[5]

1-Octyloxy-2,3-didehydro-5-methyl-oxo-pyran (**15**):



15

To a solution of Boc-pyranone **14** (5.0 g, 21.91mmol) and octan-1-ol (4.28 g, 32.9 mmol) in 30 mL of CH_2Cl_2 at 0 ˚C was added 4 Å molecular sieves (1.3 g). To this mixture was added $Pd_2(dba)_3$·$CHCl_3$ (567 mg, 2.5 mol %) and PPh_3 (576 mg, 10 mol %) solution in CH_2Cl_2. The reaction was stirred and warmed from 0 ˚C to rt. After 2 h, the reaction was quenched by adding saturated $NaHCO_3$ (30 mL), followed by extraction with Et_2O (3 x 300 mL). The organic layers were combined, washed with saturated brine solution (30 mL), dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified using silica gel flash chromatography eluting with 3-5% EtOAc/hexane to give pyranone **15** (4.9 g, 20.39 mmol, 93%): R_f (30% EtOAc/hexane) = 0.65; $\left[\alpha\right]_D^{25}$ = + 33.8 (*c* = 0.39, CH_2Cl_2); IR (thin film, cm^{-1}) 2928, 2857,1733, 1702, 1467, 1375, 1158, 1086, 1041, 749; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.80 (dd, *J* = 10.4, 3.6 Hz, 1H), 6.01 (d, *J* = 10.0 Hz, 1H), 5.11 (d, *J* = 2.8 Hz, 1H), 4.52 (q, *J* = 6.4 Hz, 1H), 3.80 (ddd, *J* = 9.6, 7.2, 6.8 Hz,1H), 3.54 (ddd, *J* = 9.6, 7.2, 6.8 Hz, 1H), 1.57 (m, 2H) 1.33 (d, *J* = 6.4 Hz, 3H), 1.26 (m, 10H), 0.87 (d, *J* = 6.0, 6.0 Hz,3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 127.4, 93.2, 70.4, 69.7, 32.0, 29.8, 29.5, 29.4, 26.3, 22.8, 15.4, 14.3; HRMS (ESI) calcd for $[C_{14}H_{24}O_3 + H]$+: 241.1745, Found: 241.1732.

Note: *in a thesis, you should also number the molecule and assign the NMR data and major IR peaks in the text*. In a journal, this level of detail is often not required.

[5]Taken from the SI for S. O. Bajaj, E. U. Sharif, N. G. Akhmedov and G. A. O'Doherty, *Chem. Sci.,* **2014,** Advance Article.

6.0 The Appendix: NMR and Chiral Assay Data of Key Compounds

In the appendix, all *NMR data* for significant **organic compounds** should be included:

- The compounds should be in numerical order, that they may be easily located by anybody trying to find them who is unfamiliar with the thesis.
- In the caption, list the field strength of the magnet, solvent, and the temperature if relevant (for example, '500MHz, $CDCl_3$, 270K');
- Proton scale typically from –0.5 to 10 ppm, but may need a larger chemical shift range if you record resonances above 10 and below 0 ppm;
- Carbon scale from –5 to 220 ppm (or higher if you have a peak above 220 ppm);
- Peaks should be picked and labelled on the top of the spectrum;
- Integration should be included for the proton spectrum;
- A picture of the molecule and its corresponding number should be included to help identify the compound you are referring to (ACS settings are recommended but whatever you choose, make sure it is consistent throughout);
- A window with enlarged sections of the spectrum should be included where it is useful in seeing splitting patterns;
- If you are reporting two-dimensional data (COSY, NOESY etc) carefully label key connectivities and include a chemical structure labelled accordingly.

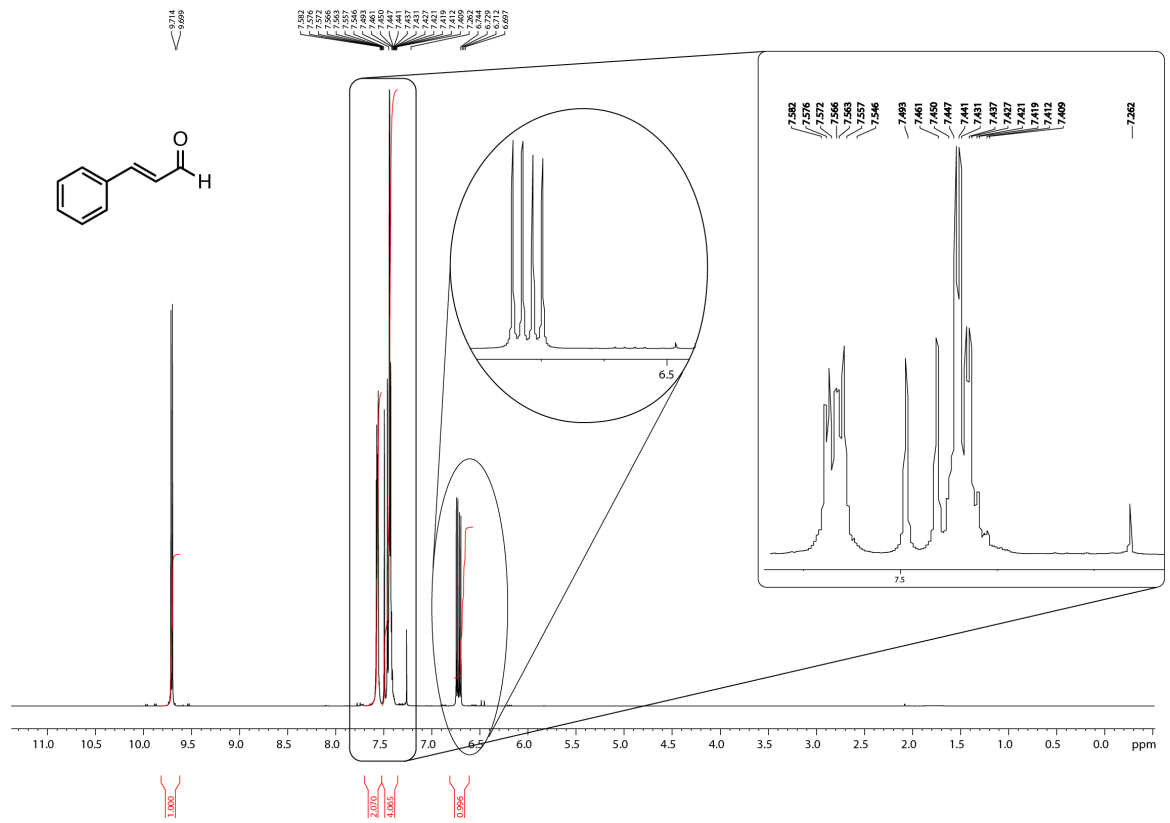
Experimentalists who find that their experimental section is taking you over the 12,000 word count should retain only the key compounds in the Experimental Section (part of the main report body, i.e. included in the word count); all other compounds (including preparation method and experimental data) should be moved to an Appendix entitled 'Supporting Information', i.e. rendering them excluded from the word count. Further information about the first year report submission can be found at: https://www.ch.cam.ac.uk/gradstudents/phd-first-year-probationary-review.

Chiral assay data should also be included for enantioselective reaction processes and labelled with a picture of the molecule and its corresponding number.

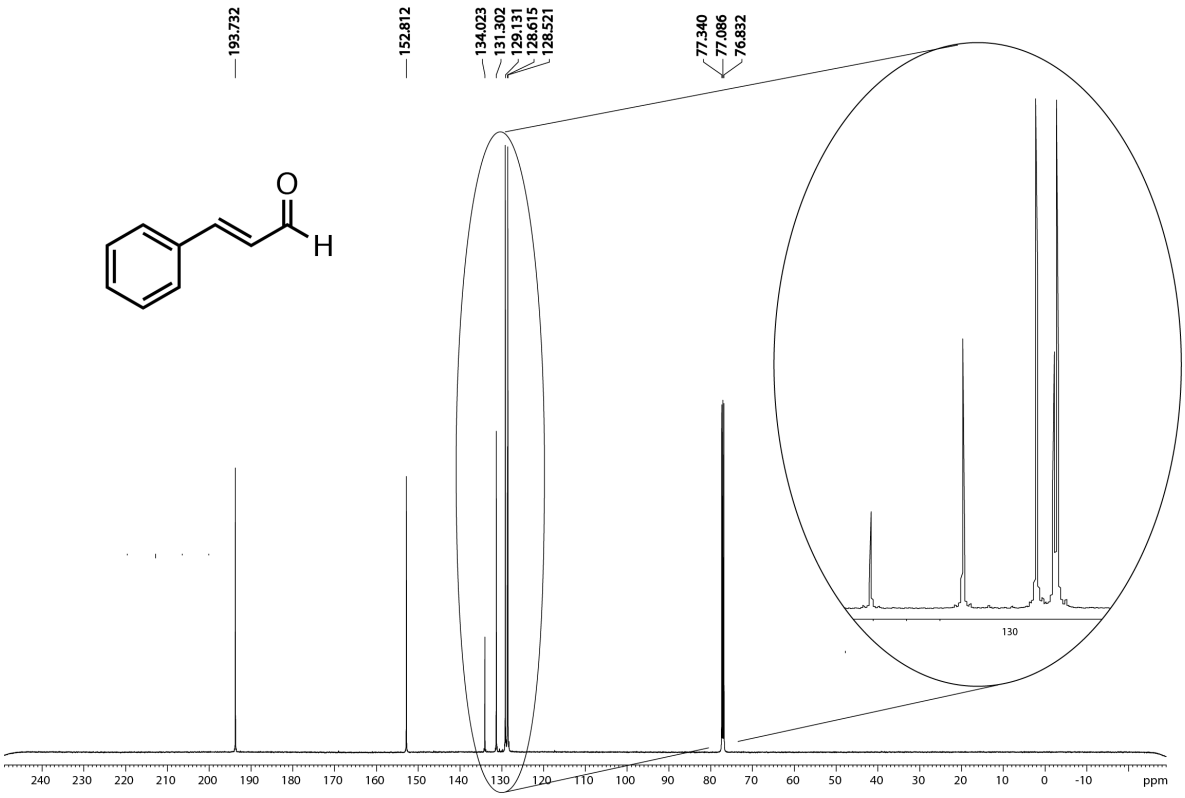
For **inorganic compounds**, all *crystal structure data* should be included in the appendix. Spectra are only included if there is something of note regarding them or if specific NMR experiments have been run. The compound structure is not required to be pasted onto spectra included in the appendix.

7.0 Example of How to Present ^{1}H and ^{13}C Data in the Appendix[6]

(2E)-3-phenylprop-2-enal (**132**)



(2E)-3-phenylprop-2-enal (**132**)



[6]Thanks to Mark Hudson for providing this data as an example.

8.0 Standard Abbreviation Checklist

You will almost certainly not use all the abbreviations on this checklist (taken from the ACS *Organic Letters* Guidelines for Authors) but when you do use an abbreviation, it is worth making sure that a) you are using the recognised standard and b) it is definitely featuring on your 'Abbreviations' page.

α	observed optical rotation in degrees	DCC	*N,N'*-dicyclohexylcarbodiimide
[α]	specific rotation [expressed without units; the units, (deg mL g^{-1} dm^{-1}), are understood]	DCE	1,2-dichloroethane
Å	angstrom(s)	DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
Ac	acetyl	DEAD	diethyl azodicarboxylate
acac	acetylacetonate	DEPT	distortionless enhancement by polarization transfer
ADP	adenosine 5'-diphosphate	DFT	density functional theory
AIBN	2,2'-azobisisobutyronitrile	DIBALH	diisobutylaluminum hydride
AM1	Austin model 1	DMA	dimethylacetamide
AMP	adenosine 5'-monophosphate	DMAP	4-(*N,N*-dimethylamino)pyridine
Anal.	combustion elemental analysis	DMDO	dimethyldioxirane
anhyd	anhydrous	DME	1,2-dimethoxyethane
AO	atomic orbital	DMF	dimethylformamide
aq	aqueous	DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
Ar	aryl	DMSO	dimethyl sulfoxide
atm	atmosphere(s)	DMT	4,4'-dimethoxytrityl (4,4'-dimethoxyltriphenylmethyl)
ATP	adenosine 5'-triphosphate	DNA	deoxyribonucleic acid
ATPase	adenosinetriphosphatase	DPS	*tert*-butyldiphenylsilyl
av	average	dp / d.p.	decimal place
9-BBN	9-borabicyclo[3.3.1]nonyl	dr	diastereomeric ratio
9-BBN–H	9-borabicyclo[3.3.1]nonane	DTT	dithiothreitol
Bn, Bzl	benzyl	E1	unimolecular elimination
bpy	2,2'-bipyridyl	E2	bimolecular elimination
BOC, Boc	*tert*-butoxycarbonyl	ED_{50}	dose effective in 50% of test subjects
bp	boiling point, base pair	EDTA	ethylenediaminetetraacetic acid
br	broad (spectral)	EI	electron impact
Bu, n-Bu, ^{n}Bu	normal (primary) butyl	EPR	electron paramagnetic resonance
s-Bu, ^{s}Bu	*sec*-butyl	eq	equation
t-Bu, ^{t}Bu	*tert*-butyl	equiv	equivalent
Bz	benzoyl (not benzyl)	er	enantiomeric ratio
B3LYP	3-parameter hybrid Becke exchange/ Lee–Yang–Parr correlation functional	ESI	electrospray ionization
°C	degrees Celsius	Et	ethyl
calcd	calculated	FAB	fast atom bombardment
cAMP	adenosine cyclic 3',5'-phosphate	FD	field desorption

CAN	ceric ammonium nitrate	FID	flame ionization detector; free induction decay
CASSCF	complete active space self-consistent field	Fmoc	9-fluorenylmethoxycarbonyl
CASPT2	complete active space with second-order perturbation theory	FT	Fourier transform
Cat.	catalytic	g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g. gCOSY, gHMQC)
CBZ, Cbz	benzyloxycarbonyl (preferred over the abbreviation Z)	GC	gas chromatography
CC	coupled cluster	GTP	guanosine 5'-triphosphate
CD	circular dichroism	h	hour(s)
cDNA	complementary deoxyribonucleic acid	HF	Hartree–Fock
c-Hex, c-C6H11	cyclohexyl	HMBC	heteronuclear multiple bond correlation
CI	chemical ionisation; configuration interaction	HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
CIF	crystallographic information file	HMQC	heteronuclear multiple quantum correlation
CIDNP	chemically induced dynamic nuclear polarisation	HOMO	highest occupied molecular orbital
cm	centimetre(s)	HPLC	high-performance liquid chromatography
cm^{-1}	wavenumber(s)	HRMS	high-resolution mass spectrometry
cod	1,5-cyclooctadiene	HSQC	heteronuclear single quantum correlation
compd	compound	Hz	hertz
concd	concentrated	ICR	ion cyclotron resonance
concn	concentration	INDO	intermediate neglect of
COSY	correlation spectroscopy	IP	ionization potential
cot	1,3,5,7-cyclooctatetraene	IR	infrared
Cp	cyclopentadienyl	*J*	coupling constant (in NMR spectrometry)
m-CPBA	*meta*-chloroperoxybenzoic acid	k	kilo
CV	cyclic voltammetry	K	kelvin(s) (absolute temperature)
δ	chemical shift in parts per million downfield from tetramethylsilane	L	litre(s)
d	day(s); doublet (spectral); deci	LAH	lithium aluminum hydride
d	density	LCAO	linear combination of atomic orbitals
DABCO	1,4-diazabicyclo[2.2.2]octane	LD_{50}	dose that is lethal in 50% of test subjects
dansyl	5-(dimethylamino)-1-naphthalenesulfonyl	LDA	lithium diisopropylamide; local density approximation
DBN	1,5-diazabicyclo[4.3.0]non-5-ene	LFER	linear free energy relationship

DBU	1,8-diazabicyclo[5.4.0]undec-7-ene	LHMDS	lithium hexamethyldisilazane, lithium bis(trimethylsilyl)amide
DCM	is *not* the abbreviation for dichloromethane. Always write the formula for this, CH_2Cl_2.	lit.	literature value (abbreviation used with full stop)
LTMP	lithium 2,2,6,6-tetramethylpiperidide	PT	perturbation theory
LUMO	lowest unoccupied molecular orbital	PTC	phase-transfer catalysis
µ	micro	Py / py	pyridine
m	multiplet (spectral); meter(s); milli	q	quartet (spectral)
M	molar (moles per liter); mega	QSAR	quantitative structure–activity relationship
M+	parent molecular ion	RCM	ring-closure metathesis
MALDI	matrix-assisted laser desorption ionization	redox	reduction–oxidation
max	maximum	rel	relative
MCD	magnetic circular dichroism	R_f	retention factor (in chromatography)
MCR	multicomponent reaction	RHF	restricted Hartree–Fock
MCSCF	multi-configuration self-consistent field	ROESY	rotating frame Overhauser effect spectroscopy
MD	molecular dynamics	ROMP	ring-opening metathesis polymerization
Me	methyl	rRNA	ribosomal ribonucleic acid
MEM	(2-methoxyethoxy)methyl	rt	room temperature
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl (mesyl)]	s	singlet (spectral); second(s)
MHz	megahertz	SAR	structure–activity relationship
min	minute(s); minimum	SCF	self-consistent field
mM	millimolar (millimoles per liter)	SEM	scanning electron microscopy
MO	molecular orbital	SN1	unimolecular nucleophilic substitution
mol	mole(s); molecular (as in mol wt)	SN2	bimolecular nucleophilic substitution
MOM	methoxymethyl	SN'	nucleophilic substitution with allylic rearrangement
mp	melting point	SOMO	single-occupied molecular orbital
MP	Møller–Plesset perturbation theory	t	triplet (spectral)
MRCI	multi-reference configuration interaction	T	time; temperature in units of degrees Celsius (˚C)
mRNA	messenger ribonucleic acid	T	absolute temperature in units of kelvins (K)
Ms	methylsulfonyl (mesyl)	TBAB	tetrabutylammonium bromide
MS	mass spectrometry	TBAC	tetrabutylammonium chloride
MTBE	methyl *tert*-butyl ether	TBAF	tetrabutylammonium fluoride
MW, mol wt	molecular weight	TBS	tert-butyldimethylsilyl

m/z	mass-to-charge ratio (not m/e)	TBHP	tert-butyl hydroperoxide
N	normal (equivalents per liter)	TCA	trichloroacetic acid
NAD+	nicotinamide adenine dinucleotide	TCNE	tetracyanoethylene
NADH	reduced NAD	TDDFT	time-dependent density functional theory
NBO	natural bond orbital	TEAB	tetraethylammonium bromide
NBS	*N*-bromosuccinimide	Temp	temperature
NCS	*N*-chlorosuccinimide	Tf	trifluoromethanesulfonyl (triflyl)
NICS	nucleus-independent chemical shift	TFA	trifluoroacetic acid
nm	nanometer(s)	TFAA	trifluoroacetic anhydride
NMO	*N*-methylmorpholine-*N*-oxide	THF	tetrahydrofuran
NMP	*N*-methylpyrrolidone	SET	single electron transfer
NMR	nuclear magnetic resonance	THP	tetrahydropyran-2-yl
NOE	nuclear Overhauser effect	TIPS	triisopropylsilyl
NOESY	nuclear Overhauser effect spectroscopy	TLC	thin-layer chromatography
NRT	natural resonance theory	TMAI	tetramethylammonium iodide
Nu	nucleophile	TMEDA	*N,N,N′,N′*-tetramethyl-1,2-ethylenediamine
obsd	observed	TMS	trimethylsilyl; tetramethylsilane
OD	optical density	TOF	time-of-flight
ORD	optical rotary dispersion	Tr	triphenylmethyl (trityl)
PCC	pyridinium chlorochromate	tRNA	transfer ribonucleic acid
PDC	pyridinium dichromate	tR	retention time (in chromatography)
PES	photoelectron spectroscopy	Ts	*p*-toluenesulfonyl (tosyl)
Ph	phenyl	TS	transition state
piv	pivaloyl	UHF	unrestricted Hartree–Fock
pm	picometer(s)	UV	ultraviolet
PM3	parametric method 3	VCD	vibrational circular dichroism
PMB	*p*-methoxybenzyl	vis	visible
PPA	poly(phosphoric acid)	vol	volume
ppm	part(s) per million	v/v	volume per unit volume (volume-to-volume ratio)
PPTS	pyridinium *p*-toluenesulfonate	wt	weight
Pr	propyl	w/w	weight per unit weight (weight-to-weight ratio)
i-Pr, ^{i}Pr	*iso*-propyl	ZINDO	Zerner parameterization of intermediate neglect of differential overlap