The Journal of Organic Chemistry

Standard Abbreviations and Acronyms

α	observed optical rotation in degrees
[α]	specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]
Å	angstrom(s)
Ac	acetyl
acac	acetylacetonate
ADP	adenosine 5′-diphosphate
AIBN	2,2′-azobisisobutyronitrile
AM1	Austin model 1
AMP	adenosine 5′-monophosphate
Anal.	combustion elemental analysis
anhyd	anhydrous
AO	atomic orbital
aq	aqueous
Ar	aryl
atm	atmosphere(s)
ATP	adenosine 5′-triphosphate
ATPase	adenosinetriphosphatase
av	average
9-BBN	9-borabicyclo[3.3.1]nonyl
9-BBN–H	9-borabicyclo[3.3.1]nonane
Bn, Bzl	benzyl
bpy	2,2′-bipyridyl
BOC, Boc	*tert*-butoxycarbonyl
bp	boiling point, base pair
br	broad (spectral)
Bu, *n*-Bu	normal (primary) butyl
s-Bu	*sec*-butyl
t-Bu	*tert*-butyl
Bz	benzoyl (not benzyl)
B3LYP	3-parameter hybrid Becke exchange/ Lee–Yang–Parr correlation functional
°C	degrees Celsius
calcd	calculated
cAMP	adenosine cyclic 3′,5′-phosphate
CAN	ceric ammonium nitrate
CASSCF	complete active space self-consistent field
CASPT2	complete active space with second-order perturbation theory
cat	catalytic
CBZ, Cbz	benzyloxycarbonyl (preferred over the abbreviation Z)
CC	coupled cluster
CD	circular dichroism
cDNA	complementary deoxyribonucleic acid
CI	chemical ionization; configuration interaction
CIF	crystallographic information file
CIDNP	chemically induced dynamic nuclear polarization
cm	centimeter(s)
cm^{-1}	wavenumber(s)
cod	1,5-cyclooctadiene
compd	compound
concd	concentrated
concn	concentration
COSY	correlation spectroscopy
cot	1,3,5,7-cyclooctatetraene
Cp	cyclopentadienyl
m-CPBA	*meta*-chloroperoxybenzoic acid
CV	cyclic voltammetry
Cy	cyclohexyl
δ	chemical shift in parts per million downfield from tetramethylsilane
d	day(s); doublet (spectral); deci
d	density
DABCO	1,4-diazabicyclo[2.2.2]octane
dansyl	5-(dimethylamino)-1-naphthalenesulfonyl
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DCC	*N,N′*-dicyclohexylcarbodiimide
DCE	1,2-dichloroethane
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DEAD	diethyl azodicarboxylate
DEPT	distortionless enhancement by polarization transfer
DFT	density functional theory
DIBALH	diisobutylaluminum hydride
DMA	dimethylacetamide
DMAP	4-(*N,N*-dimethylamino)pyridine
DMDO	dimethyldioxirane
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
DMSO	dimethyl sulfoxide
DMT	4,4′-dimethoxytrityl (4,4′-dimethoxyltriphenylmethyl)
DNA	deoxyribonucleic acid
DPS	*tert*-butyldiphenylsilyl
dr	diastereomeric ratio
DTT	dithiothreitol
E1	unimolecular elimination
E2	bimolecular elimination
ED_{50}	dose effective in 50% of test subjects
EDTA	ethylenediaminetetraacetic acid
EI	electron impact
EPR	electron paramagnetic resonance
eq	equation
equiv	equivalent
er	enantiomeric ratio
ESI	electrospray ionization
Et	ethyl
FAB	fast atom bombardment

FD	field desorption
FID	flame ionization detector; free induction decay
Fmoc	9-fluorenylmethoxycarbonyl
FT	Fourier transform
g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g. gCOSY, gHMQC)
GC	gas chromatography
GTP	guanosine 5′-triphosphate
h	hour(s)
HF	Hartree–Fock
HMBC	heteronuclear multiple bond correlation
HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
HMQC	heteronuclear multiple quantum correlation
HOMO	highest occupied molecular orbital
HPLC	high-performance liquid chromatography
HRMS	high-resolution mass spectrometry
HSQC	heteronuclear single quantum correlation
Hz	hertz
ICR	ion cyclotron resonance
INDO	intermediate neglect of differential overlap
IP	ionization potential
IR	infrared
J	coupling constant (in NMR spectrometry)
k	kilo
K	kelvin(s) (absolute temperature)
L	liter(s)
LAH	lithium aluminum hydride
LCAO	linear combination of atomic orbitals
LD_{50}	dose that is lethal in 50% of test subjects
LDA	lithium diisopropylamide; local density approximation
LFER	linear free energy relationship
LHMDS	lithium hexamethyldisilazane, lithium bis(trimethylsilyl)amide
lit.	literature value (abbreviation used with period)
LTMP	lithium 2,2,6,6-tetramethylpiperidide
LUMO	lowest unoccupied molecular orbital
μ	micro
m	multiplet (spectral); meter(s); milli
M	molar (moles per liter); mega
M^+	parent molecular ion
MALDI	matrix-assisted laser desorption ionization
max	maximum
MCD	magnetic circular dichroism
MCR	multicomponent reaction
MCSCF	multi-configuration self-consistent field
MD	molecular dynamics
Me	methyl
MEM	(2-methoxyethoxy)methyl
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl (mesyl)]
MHz	megahertz
min	minute(s); minimum
mM	millimolar (millimoles per liter)
MO	molecular orbital
mol	mole(s); molecular (as in mol wt)
MOM	methoxymethyl
mp	melting point
MP	Møller–Plesset perturbation theory
MRCI	multi-reference configuration interaction
mRNA	messenger ribonucleic acid
Ms	methylsulfonyl (mesyl)
MS	mass spectrometry
MTBE	methyl *tert*-butyl ether
MW, mol wt	molecular weight
m/*z*	mass-to-charge ratio (not *m*/*e*)
N	normal (equivalents per liter)
NAD^+	nicotinamide adenine dinucleotide
NADH	reduced NAD
NBO	natural bond orbital
NBS	*N*-bromosuccinimide
NCS	*N*-chlorosuccinimide
NICS	nucleus-independent chemical shift
nm	nanometer(s)
NMO	*N*-methylmorpholine-*N*-oxide
NMP	*N*-methylpyrrolidone
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NOESY	nuclear Overhauser effect spectroscopy
NRT	natural resonance theory
Nu	nucleophile
obsd	observed
OD	optical density
ORD	optical rotary dispersion
PCC	pyridinium chlorochromate
PDC	pyridinium dichromate
PES	photoelectron spectroscopy
Ph	phenyl
piv	pivaloyl
pm	picometer(s)
PM3	parametric method 3
PMB	*p*-methoxybenzyl
PPA	poly(phosphoric acid)
ppm	part(s) per million
PPTS	pyridinium *para*-toluenesulfonate
Pr	propyl
i-Pr	isopropyl
PT	perturbation theory
PTC	phase-transfer catalysis
py	pyridine
q	quartet (spectral)
QSAR	quantitative structure–activity relationship

RCM	ring-closure metathesis
redox	reduction–oxidation
rel	relative
R_f	retention factor (in chromatography)
RHF	restricted Hartree–Fock
ROESY	rotating frame Overhauser effect spectroscopy
ROMP	ring-opening metathesis polymerization
rRNA	ribosomal ribonucleic acid
rt	room temperature
s	singlet (spectral); second(s)
SAR	structure–activity relationship
SCF	self-consistent field
SEM	scanning electron microscopy; 2-trimethylsilylethoxymethyl
SET	single electron transfer
S_N1	unimolecular nucleophilic substitution
S_N2	bimolecular nucleophilic substitution
S_N'	nucleophilic substitution with allylic rearrangement
SOMO	single-occupied molecular orbital
t	triplet (spectral)
t	time; temperature in units of degrees Celsius (ºC)
T	absolute temperature in units of kelvins (K)
TBAB	tetrabutylammonium bromide
TBAC	tetrabutylammonium chloride
TBAF	tetrabutylammonium fluoride
TBS	*tert*-butyldimethylsilyl
TBHP	*tert*-butyl hydroperoxide
TCA	trichloroacetic acid
TCNE	tetracyanoethylene
TDDFT	time-dependent density functional theory
TEAB	tetraethylammonium bromide
temp	temperature
Tf	trifluoromethanesulfonyl (triflyl)
TFA	trifluoroacetic acid
TFAA	trifluoroacetic anhydride
THF	tetrahydrofuran
THP	tetrahydropyran-2-yl
TIPS	triisopropylsilyl
TLC	thin-layer chromatography
TMAI	tetramethylammonium iodide
TMEDA	*N,N,N′,N′*-tetramethyl-1,2-ethylenediamine
TMS	trimethylsilyl; tetramethylsilane
TOF	time-of-flight
Tr	triphenylmethyl (trityl)
tRNA	transfer ribonucleic acid
t_R	retention time (in chromatography)
Ts	*para*-toluenesulfonyl (tosyl)
TS	transition state
UHF	unrestricted Hartree–Fock
UV	ultraviolet
VCD	vibrational circular dichroism
vis	visible
vol	volume
v/v	volume per unit volume (volume-to-volume ratio)
wt	weight
w/w	weight per unit weight (weight-to-weight ratio)
ZINDO	Zerner parameterization of intermediate neglect of differential overlap