

Standard Abbreviations and Acronyms

| | | | |
|---|---|------------------|--|
| α | observed optical rotation in degrees | cm^{-1} | wavenumber(s) |
| $[\alpha]$ | specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood] | cod | 1,5-cyclooctadiene |
| Å | angstrom(s) | compd | compound |
| Ac | acetyl | concd | concentrated |
| acac | acetylacetonate | concn | concentration |
| ADP | adenosine 5'-diphosphate | COSY | correlation spectroscopy |
| AIBN | 2,2'-azobisisobutyronitrile | cot | 1,3,5,7-cyclooctatetraene |
| AM1 | Austin model 1 | Cp | cyclopentadienyl |
| AMP | adenosine 5'-monophosphate | <i>m</i> -CPBA | <i>meta</i> -chloroperoxybenzoic acid |
| Anal. | combustion elemental analysis | CV | cyclic voltammetry |
| anhyd | anhydrous | δ | chemical shift in parts per million downfield from tetramethylsilane |
| AO | atomic orbital | d | day(s); doublet (spectral); deci |
| aq | aqueous | <i>d</i> | density |
| Ar | aryl | DABCO | 1,4-diazabicyclo[2.2.2]octane |
| atm | atmosphere(s) | dansyl | 5-(dimethylamino)-1-naphthalenesulfonyl |
| ATP | adenosine 5'-triphosphate | DBN | 1,5-diazabicyclo[4.3.0]non-5-ene |
| ATPase | adenosinetriphosphatase | DBU | 1,8-diazabicyclo[5.4.0]undec-7-ene |
| av | average | DCC | <i>N,N'</i> -dicyclohexylcarbodiimide |
| 9-BBN | 9-borabicyclo[3.3.1]nonyl | DCE | 1,2-dichloroethane |
| 9-BBN-H | 9-borabicyclo[3.3.1]nonane | DDQ | 2,3-dichloro-5,6-dicyano-1,4-benzoquinone |
| Bn, Bzl | benzyl | DEAD | diethyl azodicarboxylate |
| bpy | 2,2'-bipyridyl | DEPT | distortionless enhancement by polarization transfer |
| BOC, Boc | <i>tert</i> -butoxycarbonyl | DFT | density functional theory |
| bp | boiling point, base pair | DIBALH | diisobutylaluminum hydride |
| br | broad (spectral) | DMA | dimethylacetamide |
| Bu, <i>n</i> -Bu | normal (primary) butyl | DMAP | 4-(<i>N,N</i> -dimethylamino)pyridine |
| <i>s</i> -Bu | <i>sec</i> -butyl | DMDO | dimethyldioxirane |
| <i>t</i> -Bu | <i>tert</i> -butyl | DME | 1,2-dimethoxyethane |
| Bz | benzoyl (not benzyl) | DMF | dimethylformamide |
| B3LYP | 3-parameter hybrid Becke exchange/Lee-Yang-Parr correlation functional | DMPU | 1,3-dimethyl-3,4,5,6-tetrahydro-2(1 <i>H</i>)-pyrimidinone |
| °C | degrees Celsius | DMSO | dimethyl sulfoxide |
| calcd | calculated | DMT | 4,4'-dimethoxytrityl (4,4'-dimethoxytriphenylmethyl) |
| cAMP | adenosine cyclic 3',5'-phosphate | DNA | deoxyribonucleic acid |
| CAN | ceric ammonium nitrate | DPS | <i>tert</i> -butyldiphenylsilyl |
| CASSCF | complete active space self-consistent field | dr | diastereomeric ratio |
| CASPT2 | complete active space with second-order perturbation theory | DTT | dithiothreitol |
| cat | catalytic | E1 | unimolecular elimination |
| CBZ, Cbz | benzyloxycarbonyl (preferred over the abbreviation Z) | E2 | bimolecular elimination |
| CC | coupled cluster | ED ₅₀ | dose effective in 50% of test subjects |
| CD | circular dichroism | EDTA | ethylenediaminetetraacetic acid |
| cDNA | complementary deoxyribonucleic acid | EI | electron impact |
| <i>c</i> -Hex, <i>c</i> -C ₆ H ₁₁ | cyclohexyl | EPR | electron paramagnetic resonance |
| CI | chemical ionization; configuration interaction | eq | equation |
| CIF | crystallographic information file | equiv | equivalent |
| CIDNP | chemically induced dynamic nuclear polarization | er | enantiomeric ratio |
| cm | centimeter(s) | ESI | electrospray ionization |
| | | Et | ethyl |
| | | FAB | fast atom bombardment |

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

| | | | |
|--------|---|-------|--|
| RCM | ring-closure metathesis | vis | visible |
| redox | reduction–oxidation | vol | volume |
| rel | relative | v/v | volume per unit volume (volume-to-volume ratio) |
| R_f | retention factor (in chromatography) | | |
| RHF | restricted Hartree–Fock | wt | weight |
| ROESY | rotating frame Overhauser effect spectroscopy | w/w | weight per unit weight (weight-to-weight ratio) |
| ROMP | ring-opening metathesis polymerization | ZINDO | Zerner parameterization of intermediate neglect of differential overlap |
| rRNA | ribosomal ribonucleic acid | | |
| rt | room temperature | | |
| s | singlet (spectral); second(s) | | |
| SAR | structure–activity relationship | | |
| SCF | self-consistent field | | |
| SEM | scanning electron microscopy | | |
| 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 ($^{\circ}\text{C}$) | | |
| T | absolute temperature in units of kelvins (K) | | |
| TBAB | tetrabutylammonium bromide | | |
| TBAC | tetrabutylammonium chloride | | |
| TBAF | tetrabutylammonium fluoride | | |
| TBS | <i>tert</i> -butyldimethylsilyl | | |
| TBHP | <i>tert</i> -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 | <i>N,N,N',N'</i> -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 | <i>para</i> -toluenesulfonyl (tosyl) | | |
| TS | transition state | | |
| UHF | unrestricted Hartree–Fock | | |
| UV | ultraviolet | | |
| VCD | vibrational circular dichroism | | |