

Nomenclature: Chemical nomenclature, abbreviations and symbols must follow IUPAC rules. Whenever possible, avoid coining new trivial names; **every effort should be made to modify an existing name**. For example, when a new compound is described, it should be given a full systematic name according to IUPAC nomenclature and this should be cited in the Abstract or in the Experimental section. Isotopically-labeled substances should be written with the correct chemical name of the compound. The symbol for the isotope should be placed in square brackets and should precede that part of the name to which it refers, e.g. sodium [¹⁴C]formate.

Optical rotation, optical rotary dispersion, circular dichroism. Data should be presented in the established form, e.g.

$[\alpha]_D^{temp.}$ Value (+ or -) in ° (solvent used; $c \left\{ \frac{Wt \text{ of compound}}{100ml \text{ solvent}} \right\}$)

Example: $[\alpha]_D^{23} + 32^\circ(\text{EtOH}; c 0.3210)$.

ORD curves are usually described as a series of values based on $[\alpha]$ or $[\theta]$ (molecular rotation) at various wavelengths.

CD values may be expressed as molecular ellipticity values $[\theta]$, e.g., $[\theta]_{256} + 21\ 780$, $[\theta]_{307} - 16\ 113$ or as differential dichroic absorption, e.g. $\Delta\varepsilon_{253} - 1.0$ (MeOH; $c\ 0.164$).

Ultraviolet-visible Spectra: ε values are give as log values in parentheses, e.g. λ_{\max}^{EtOH} nm (log ε): 203 (4.7), etc.

Infrared spectra: Data should be presented in the established form, e.g.

$\nu_{\max}^{\text{CHCl}_3}$ cm^{-1} : 1740, etc.

Absorption should be expressed only in wave-numbers and structural assignments should be indicated when possible in parenthesis after the relevant wave-number, e.g. 1740 (>C=O), etc. The following abbreviations should be used if the intensity of absorption bands are included: w-weak intensity, m-medium intensity, v-variable intensity, s-strong intensity, vs-very strong intensity.

NMR spectral data should only be presented in full if they have not been published separately elsewhere in which case only relevant references should be quoted. Data must be specified as ¹H NMR or ¹³C NMR and should indicate the frequency of the instrument, the solvent used and the internal standard. Chemical shifts should be quoted in δ units relative to TMS with indication of whether the signal is a singlet *s*, doublet *d*, doublet of doublets *dd*, triplet *t*, multiplet *m*, etc. ¹³C NMR spectral data should specify the carbon concerned, using the recommended IUPAC numbering (e.g. C-1, C-2), and should be given to one decimal place. ¹H NMR spectral data should indicate the number of hydrogens involved and their position of attachment based on the numbering of the carbon atoms, preferably according to IUPAC rules. For example- ¹³C NMR spectral data (25.15 MHz, CDCl₃): δ 30.1 (*t*, C-5), 74.1 (*d*, C-6), 121.7 (*d*, C-3), 144.2 (*s*, C-4), etc. ¹H NMR spectral data (100 MHz, CDCl₃): δ 0.68 (3H, *s*, H-18), 0.88 (6H, *d*, $J = 6$ Hz, H-26 and H-27), 0.90 (3H, *d*, $J = 5$ Hz, H-21), 4.34 (1H, *q*, $J_{6\alpha,7\alpha} = 4.5$ Hz, $J_{6\alpha,7\beta} = 2$ Hz, H-6), 4.21 (1H, *m*, $W_{1/2} = 18$ Hz, H-3 α).

Mass spectral data should only be presented in full if they have not been published separately elsewhere, in which case only relevant references should be quoted. Presentation of mass spectral data should in general follow the recommendations given in Int. J. Mass Spectrom. Ion Processes, 142, 211-240 (1995) and must indicate the method used (EIMS, CIMS, GC-MS, etc.) and the ionizing energy. The data should give only diagnostically important ions, the character of the fragmentation ions in relation to the molecular ion and the intensity relative to the major ion. For example-EIMS (probe) 70 eV, m/z (rel. int.): 386 $[M]^+$ (36), 368 $[M-H_2O]^+$ (100), 353 $[M-H_2O-Me]^+$ (23), 275 $[M-111]^+$ (35), etc. CIMS (*iso*-butane, probe), 200eV, m/z (rel. int.): 387 $[M+H]^+$ (100), 369 $[(M+H)-H_2O]^+$ (23), etc. High-resolution spectra can be given in more detail if necessary for $[M]^+$ and the more important fragment ions.

Thin-layer chromatography

(a) For analytical TLC, dimensions of the plates can be deleted if layer thickness is 0.25 mm.

(b) Abbreviate common adsorbents: (but use silica gel, not SiO₂ as this does not describe the material accurately), Al₂O₃ (alumina).

(c) Preparative forms of the technique should include details of (i) layer thickness (prep. TLC only), (ii) amount of sample applied to the layer, (iii) method of detection used to locate the bands and (iv) the solvent used to recover the compounds from the adsorbent after development.

(d) Special forms of TLC on impregnated adsorbents can be abbreviated, e.g. AgNO₃-silica gel (1:9), by wt can be assumed.

Gas chromatography

- (a) Detector used should be specified, e.g. dual FID, EC, etc.
- (b) Carrier gas and flow rate should be given, e.g. N₂ at 30 ml min⁻¹.
- (c) Operating conditions such as injector and detector heater temps. etc., should be included.
- (d) Packed columns, e.g. 6 m × 3 mm (i.d. measurement only) packed with 1 % SE-30 (support material and mesh size can be omitted unless unusual).
- (e) Capillary columns should be specified, e.g. WCOT (wall coated open tubular), SCOT (support coated open tubular). The split ratio used in the injection system and the injection vol. for the sample should also be included.

High performance liquid chromatography

- (a) Solvent or solvent gradients used together with flow rate should be given.
- (b) Column dimensions (length × i.d. only) and packing used.
- (c) Method of detection employed, e.g. UV or refractive index.