

Specimen of Writing Up for the Experimental Section of Theses or Reports

(12 point Times, double spaced, not justified, no indents, super - and subscripts 10 point, 3 points up and 2 down, respectively)

Separate line, all bold. Capital letter for first word only

Structure here optional but helpful

Include provenance of starting material. Change to reference at last stage of writing up or use EndNote

(1R, 2R)-1,2-Bis(3-fluorophenyl)-1,2-dimethoxyethane XXX

No indent, separate line

Space before units

Shift-Option-8

Note a space is needed here

(1R, 2R)-1,2-Bis(3-fluorophenyl)ethane-1,2-diol^{XX} **XXX** (4.31 g, 17.2 mmol) was dissolved in dry THF (20 ml) and added *via* cannula to a stirred suspension of sodium hydride 60% wt. (2.36 g, 59.0 mmol) in dry THF (200 ml) at 2 °C under argon. Residual diol was added with more THF (20 ml). The reaction mixture was stirred and allowed to reach room temperature. It was stirred for 1 h, cooled to 2 °C, and methyl iodide (2.30 ml, 36.9 mmol) added dropwise. The mixture was allowed to come to room temperature and stirred overnight before sodium hydroxide solution (45 ml, 2.9 M) was added. The mixture was vigorously stirred for 3 h. The layers were separated and the aqueous layer extracted with Et₂O (3 × 100 ml). The combined organic extracts were evaporated and water removed as an azeotrope with toluene (2 × 200 ml). The residue was purified by flash chromatography, eluting with 1:1 Et₂O-hexane, to give the *diether* (4.71 g, 98.3%) as needles, mp 88-88.5 °C (from Et₂O-hexane); *R*_f(Et₂O-hexane, 1:1) 0.50; *v*_{max} (CHCl₃)/cm⁻¹ 2828 (OC-H), 1614 (Ar) and 1592 (Ar); *δ*_H(400 MHz; CDCl₃) 7.12 (2 H, td, *J* 8.0 and ⁴*J*_{HF} 5.9, 5-ArH), 6.88 (2 H, tdd, ³*J*_{HF} 8.6, *J* 8.6, 2.5 and 0.8, 4-ArH), 6.79-6.73 (4 H, m, 2 and 6-ArH), 4.27 (2 H, s, ArCH) and 3.27 (6 H, s, OMe); *δ*_C(100.6 MHz; CDCl₃) 163.0⁻ (¹*J*_{HF} 204.6, 3-ArC), 140.9⁻ (1-ArC), 129.6⁺ (³*J*_{HF} 7.8, 5-ArC), 123.7⁺ (6-ArC), 114.9⁺ (²*J*_{HF} 21.2), 114.6⁺ (²*J*_{HF} 21.9), 86.9⁺ (ArCH) and 57.5⁺ (Me); *δ*_F(235.4 MHz; CDCl₃; ¹H Decoupled) -113.9; *m/z* (EI) 247 (4.5%, M - OMe) and 139 (100, ArCHOMe)(Found: C, 69.1; H, 5.80). C₁₆H₁₆F₂O₂ requires C, 69.1; H, 5.80); [*α*]_D²⁴ -50.8 (*c* 0.985 in CH₂Cl₂).

Bold number. Convert to final number at last stage of writing up. No brackets

Avoid construction: "To the...was added"

Where possible use the same number of sig. fig. for calculations as for measurements

Perkin prefers cm³ to ml.

10 Point

Yield of recrystallised material or of material used in next step

Or plates or cubes but not crystals

Largest coupling first. Triplet is 8.0 Hz and doublet is 5.9 Hz

Perkin prefers 5-H

Italic H only when ambiguous otherwise

(Option -) for Minus -

Quote only assignable or strong peaks in MS

Symbol Font Option-y

Italic only when it is a new compound

Or film / KBr / Nujol

Quote only assignable peaks in IR

Quote all peaks in NMR. Avoid m unless it's really an indecipherable multiplet

From APT, - for even number of attached protons + for odd

Do not guess assignments - it's bad science

Keep reference near to where it refers until last stage of writing up or use EndNote

Command [Backslash]O(²⁴,_D) to achieve this. No "°" here

Italic

Round C, H, N to nearest 0.1% (or 0.05% for H)

Perkin prefers cm³ to ml.

10 Point

Yield of recrystallised material or of material used in next step

Or plates or cubes but not crystals

Largest coupling first. Triplet is 8.0 Hz and doublet is 5.9 Hz

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Italic H only when ambiguous otherwise

(Option -) for Minus -

Quote only assignable or strong peaks in MS

XXI. I. Lapkin, T. N. Povarnitsyna and L. A. Kosareva, *Zh. Obshch. Khim.*, 1969, **39**(7), 1460.

Known compounds: ... diether^{XX} (4.71 g, 98.3%) as needles, mp 88-88.5 °C (from Et₂O-hexane)(lit.,^{XX} 89-90 °C). If the product is coloured then give its colour but there is no need to say that it's colourless. All new compounds need either a combustion analysis (correct to ±0.3%) or a high resolution MS. Many journals insist on combustion analysis. Known compounds do not need either. A racemic diastereomer: **(1RS, 2RS)-1,2-Bis(3-fluorophenyl)-1,2-dimethoxyethane**. Brackets within brackets {[()]} . IUPAC name of compound must be somewhere, either in the heading or at the point where *diether* is in the example above. Convert all Symbol font to 11pt when finished.