How to write a scientific report

A short guideline to write efficient scientific reports

Oral and written communications are increasingly important in the scientific world. For this reason, great care will be taken during these practical sessions to learn basic notions for writing scientific reports. One report is due after the monostep synthesis (the week following the end of the experiment) and a second report is due at the end of the multistep synthesis (one week after the end of the practical sessions). The results of the analytical studies should be indicated in one of the two reports.

I- General remarks

Language

As scientific communications (publications, lectures) are mostly given in English, we encourage you to write your reports in English. Care has to be taken to favor short sentences and to avoid repetitions. Scientific reports do not contain emotional comments. Plagiarism (copying from publications or reports from other persons) is absolutely forbidden. Any reference to published resources has to be clearly indicated.

Preferred style for text: Arial, Times New Roman, Calibri (10-12); Bold/italics/underlined can be used for titles of chapters and subchapters and/or to emphasize parts of the text. The text should be justified.

Illustrations

All illustrations must have a title (brief title, a few words) and are classified as:

Figure: no reaction arrow (reaction equipment)

Equation*:* ONLY one reaction arrow (reaction equation)

Scheme: more than one reaction arrow (mechanism drawing, multi-step synthetic sequence)

Tables

The use of table is recommended to present a collection of data related to the same reaction (reaction scope, optimization, conditions screening). A table is also used to present quantities/properties of reagents and solvents.

Numbering the structures

All the exactly defined structures (meaning without general R or X) are numbered in order of appearance in the main text using arabic numbers. Reactive intermediates and transition states are numbered with roman numbers or letters (starting from I or A) in each new illustration. This is particularly useful when drawing mechanism intermediates.

II- Structure of the report

Title page

It includes the title of the work, main information about the course, generalities of the candidate (see Template). For long reports, table of content and list of abbreviations are given.

Introduction

It should include a scheme of the reaction (preferably made with ChemDraw in ACS style), a brief explanation about the experiment and references from the literature. Only the type of reaction is cited here (nucleophilic substitution, elimination, cycloaddition, electrophilic addition, etc). The mechanism is discussed in another section of the report.

Example: The electrophilic addition of double bonds to strong acids of type HX is a classical reaction in organic synthesis to generate halogenated compounds from olefins. It follows the Markovnikov's rule affording the more substituted halogenated isomer.

Mechanisms

Reaction mechanisms are represented with drawing softwares such as ChemDraw (ACS style). Reactivity arrows represent the moving of electrons (from nucleophile to electrophile). You should check that charges are balanced within species at each step of the mechanism. When a catalyst is used, it should be regenerated in the reaction mechanism. Full arrows (→) stand for normal reactivity and half arrows stand for radical transformations.

Experimental part

Table of reactants.

All reactant must be written with correct molecular weight, equivalents, mass, density and volume (when required). Safety risk symbols must be notified. It does not mean that the whole list that you find on the database should be indicated: 1-2 at the maximum and within the most relevant. The risk symbol has the purpose to warn you on how to handle/threat/behave with that specific chemical. Solvents (the ones used for the reaction only; solvents used for the work-up are not listed here) are placed at the bottom of the table.

Procedure. Description of the procedure should be concise and precise in order to allow someone else to repeat the same experiment. The reactants must be indicated by their IUPAC name or common name followed by quantitative data in parenthesis (moles (mol or mmol), equivalents (eq.), mass (g) or volume (mL)). The solvent must be written either as its common acronym or in the extended form followed by the amount in parenthesis (mL). Temperature (in °C) and time should be clearly indicated. If the ones that you use are different from the reported procedure, indicate the ones that you experienced. The method used to monitor the reaction [thin layer chromatography (TLC, eluent, stain, R_f) or NMR (frequency in MHz, solvent) or GC/MS (Column Name, length, diameter, oven program, retention time) or HPLC (Column Name, length, diameter, eluent, gradient if relevant, retention time), etc] has to be indicated.

The work-up procedure is then described, indicating the quenching solution (name and volume in parenthesis), the extraction solvent(s) (name and volume in parenthesis) and the number of extractions. The washing solutions are also indicated (name and volume in parenthesis), followed by name of the drying agent (if used) and method performed to obtain the crude product (for example:

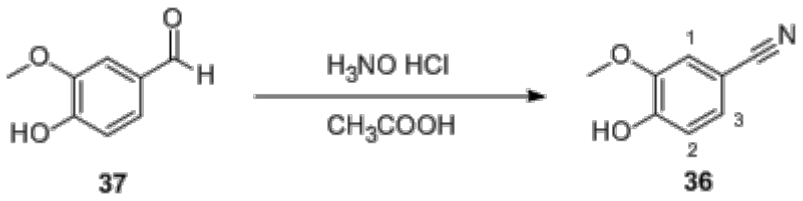
concentration under reduced pressure). Characteristics of the crude product can be indicated there [physical state (solid, or liquid, or oil), color, mass]

The purification procedure is then clearly described: (i) in case of distillation: type and height of column, pressure, T Eb in °C; (ii) in case of adsorption chromatography: name of stationary phase, eluent, R_f of isolated product; (iii) in case of recrystallization: solvent and quantity (mL).

Characteristics of the isolated product(s) are indicated: physical state, color, mass (g), yield (%).

Example.

Synthesis of 4-hydroxy-3-methoxybenzonitrile



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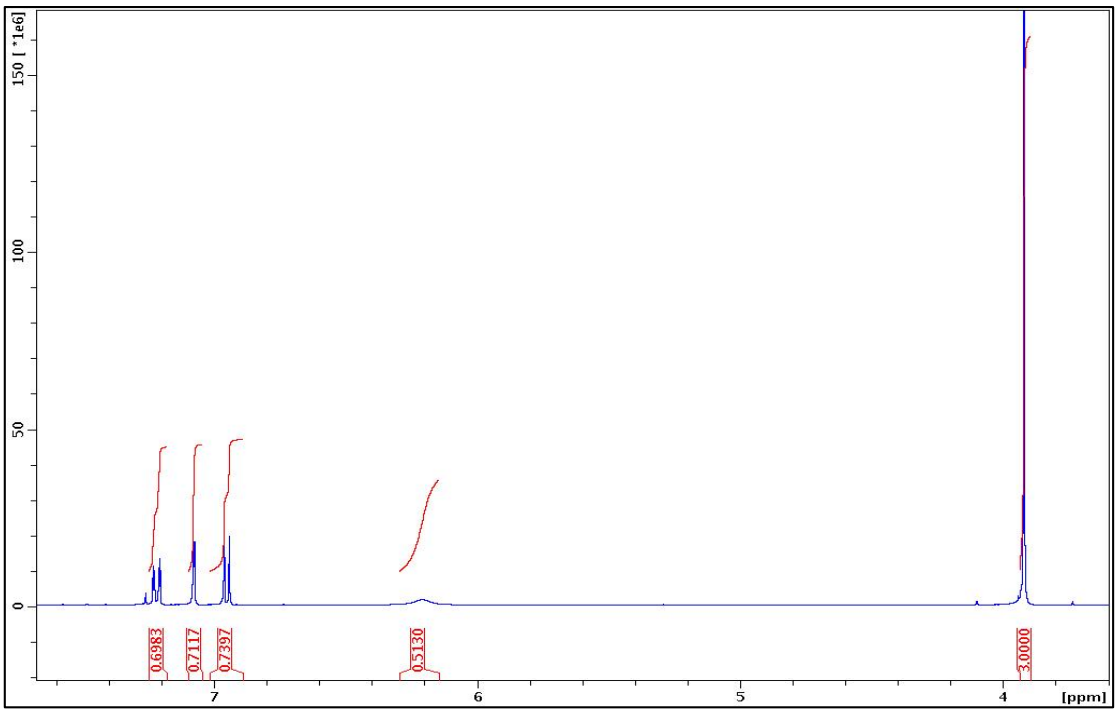
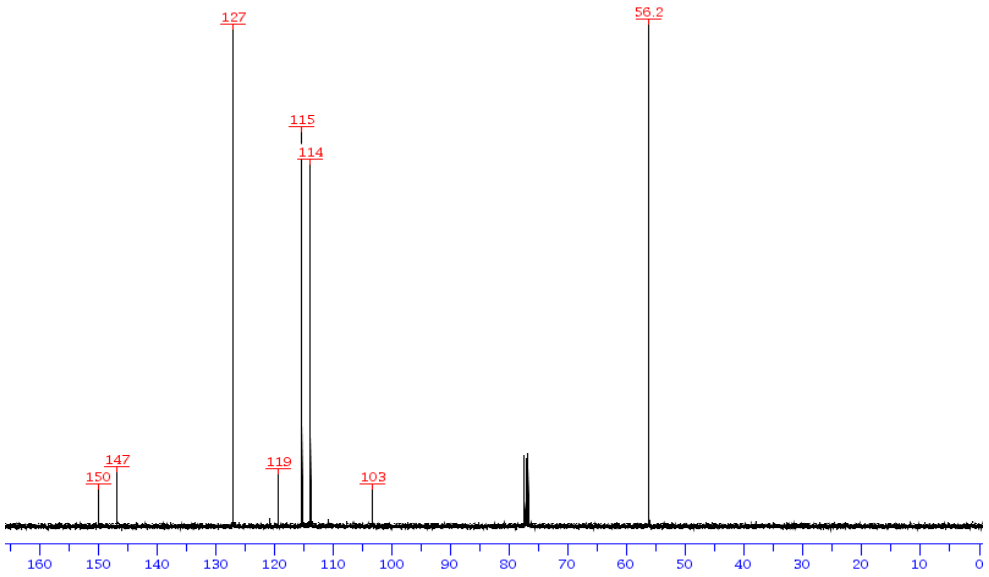
To a solution of vanillin (50.33 mmol, 1 eq., 7.66 g) in acetic acid (60 mL) was added hydroxylamine hydrochloride (75.5 mmol, 1.5 eq., 5.25 g). The solution was stirred at reflux for 90 min. The reaction was monitored by TLC PET/AcOEt 1:1 R_f: 0.67. Then the reaction mixture was cooled to room temperature and diluted with Et_2O (300 mL). The solution was washed with water (300 mL) and brine (3x100 mL). The organic layer was dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash column chromatography (petroleum ether/AcOEt 3:1) to afford **36** as a slightly yellow solid (49.4 mmol, 7.37 g, 98 % yield). **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 7.21 (dd, 1H, *J*= 8.2, 1.8 Hz, **H**3), 7.07 (d, 1H, J= 1.8 Hz, **H**1), 6.95 (d, 1H, J= 8.2 Hz, **H**2), 6.20 (s, 1H, **H**O), 3.92 (s, 3H, C**H**$_3$-O). **^{13}C-NMR (101 MHz, $CDCl_3$)** δ 150.0 (C_{ar}), 146.7 (C_{ar}), 127.0 (CH_{ar}), 119.3 (C), 115.3 (CH_{ar}), 113.8 (CH_{ar}), 103.3 (C_{ar}), 56.3 (CH_3). **Elemental Analysis** for $C_8H_7NO_2$ (%): C 64.42, H 4.73, N 9.39; found: C 64.03, N 9.26, H 4.59. **IR :** 3360, 2940, 2225, 1590, 1510, 1280, 1030, 795.

^{1}H-NMR spectrum of **36**



^{13}C-NMR spectrum of **36**



Results and discussion

This section contains analysis of the product (purity, yield compared with literature data if available) and discussion of the reaction procedure. Copies of NMR, MS and IR spectra are included as Annex to the report. Any problems encountered during the reaction development, in any of its parts must be discussed here. The procedure that you tried to overcome these problems should be explained.

Example

The product did not distilled at the expected temperature. Why?

The product did not crystallize. Why?

Purity is not satisfactory after all the manipulations. Why?

Conclusion

It is a summary of the experience. You have to recall to the reader what type of reaction was performed, the success or not of the experience (how much of the product you have obtained and with what purity), eventual major inconvenient encountered during the experience, any suggestion to give to overcome the problems.

Signature

Date of completion of the report and signature of the author should be included at the end of the document.