Advanced tabulation of a multitude of spectra is best done by combining ${ }^{1} \mathrm{H}$-based data separately from ${ }^{13} \mathrm{C}$-based data. These examples are more sophisticated than the tables you've previously completed. Not all data columns apply to every problem, so eliminate any blank columns when you re-write this information into your report.

Table 1: ${ }^{1} \mathrm{H}$ and COSY NMR of ethanol in $\mathrm{CDCl}_{3}$ (see appendices 1-2)

| Shift $(\mathrm{ppm})$ multiplicity, <br> coupling $(\mathrm{Hz})$, relative integration | COSY shows correlation <br> to protons at $\delta(\mathrm{ppm})$ | Assignment | Reference Values |
| :--- | :--- | :--- | :--- |
| $1.27 \mathrm{t},{ }^{3} \mathrm{~J}_{\mathrm{AB}}=7,3 H$ | $3.7\left(\mathrm{H}_{\mathrm{B}}\right)$ | A | $1.2 \mathrm{t}^{2}$ |
| 1.51 s | - | water in $\mathrm{CDCl}_{3}$ | $1.56^{1}$ |
| $3.73 \mathrm{q},{ }^{3} \mathrm{~J}_{\mathrm{BA}}=7,2 \mathrm{H}$ | $1.3\left(\mathrm{H}_{\mathrm{A}}\right)$ | B | $3.7 \mathrm{~m}^{2}$ |
| $3.90 \mathrm{~s}, 1 \mathrm{H}$ | - | C | $3.4 \mathrm{t}^{2}$ |
| 7.24 s | - | $\mathrm{CHCl}_{3}$ in $\mathrm{CDCl}_{3}$ | 7.261 |



A diagram of the molecule should be on the same page as the data table(s). Repeat the diagram if tables span several pages; facing page is sufficient if report is printed 2-sided.

Table 2: ${ }^{13} \mathrm{C}$, DEPT-135 and 2D NMR of ethanol in $\mathrm{CDCl}_{3}$ (see appendices 3-6)

| Shift (ppm) multiplicity, coupling (Hz), DEPT phase | 2D spectra shows correlation to protons at $\delta(\mathrm{ppm})$, assignment |  | Assignment | Reference Values |
| :---: | :---: | :---: | :---: | :---: |
|  | HMQC ( ${ }^{1} \mathrm{~J}_{\mathrm{CH}}$ ) | $\operatorname{HMBC}\left({ }^{3} \mathrm{~J}_{\mathrm{CH}}\right)$ |  |  |
| 18.42 s , $\uparrow$ | $1.3, \mathrm{H}_{\mathrm{A}}$ | $3.9, \mathrm{H}_{\mathrm{C}}$ | a | $18.13{ }^{3}$ |
| 58.34 s, | 3.7, $\mathrm{H}_{\mathrm{B}}$ | - | b | $57.79{ }^{3}$ |
| $77.11 \mathrm{t},{ }^{1} \mathrm{~J}_{\mathrm{CD}}=32, \mathrm{x}$ | - | - | $\mathrm{CDCl}_{3}$ | $77.16^{1}$ |

DEPT phase legend: $\uparrow$ positive, $\downarrow$ negative, x absent
References:

1. Chem 213 manual, University of Victoria, 2018, pages 76-79.
2. Sigma-Aldrich, http://www.sigmaaldrich.com/spectra/fnmr/FNMR004114.PDF, June 18, 2019
3. SDBS, https://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi, June 18, 2019

Appendices:
A list of appendices is not required, but a number and title should appear at the top of the first page of each appendix; subsequent pages within that appendix do not need a title.

1. ${ }^{1} \mathrm{H}$ NMR of ethanol (include original spectrum and relevant expansions)
2. COSY NMR of ethanol
3. ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}$ NMR of ethanol (include original spectrum and relevant expansions)
4. DEPT-135 NMR of ethanol (include original spectrum and relevant expansions)
5. HMQC NMR of ethanol
6. HMBC NMR of ethanol
