Notes on Thesis Corrections

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General

I have made some stylistic changes to the thesis (specifically, the formatting of the title page and chapter titles). Ralph asked about Oxford formatting guidelines. I am unaware of Oxford having specific thesis format guidelines, and haven't been able to find any guidance on this, so I am assuming that my thesis format is acceptable.

Spaces were added to citations.

In the corrected thesis, corrections which aren't simply typo fixes are in red.

Corrections by page

Page 3 – Specified that only nuclei with odd numbers of protons and/or neutrons possess spin.

Page 3 – Mentioned molecular rotation as an additional source of angular momentum.

Page 3 – Equation 1.1: Squared the reduced Planck constant.

Page 3 – Replaced "with non-zero spin" with "with spin".

Page 4 – Table 1.1: Updated caption to include source of gyromagnetic ratios.

Page 4 – Replaced "which are spin-0" with "which do not possess spin".

Page 5 – Figure 1.1: Mentioned the sign of γ for each nucleus in the caption.

Page 6 – Mentioned that the high temperature approximation is applied in arriving at Equation 1.8. See also Footnote ‡.

Page 7 – Re-worded description of RF pulse. See also Footnote ‖.

Page 7 – Equation 1.13: Corrected the expressions for $\tilde{i}$ and $\tilde{j}$.

Page 8 – Included a more detailed qualitative description of relaxation.

Page 10 – Explicitly mentioned the presence of a vacuum chamber.

Page 10 – Included solid-state NMR as an area that requires very high field strengths.

Page 11 – "inhomogeneities" → "small inhomogeneities".

Page 11 – A few extra details about the probe.

Page 12 – "is sent to" → "travels to".

Page 12 – Peter suggested that I mention how data could be treated if there were line-shape distortions (annotation on Section 3.1.2 heading). Footnote ‡‡ mentions reference deconvolution as a means of correcting these in order to yield Lorentzian lineshapes.

Page 12 – Replace "sweep width" with "spectral width". This has been done in numerous places in the thesis.

Page 13 – Equation 1.18b: Correct equation label.

Page 17 – Mentioned that exponential broadening is not the optimal window function for sensitivity enhancement. See also Footnote ¶¶.

Page 17 – Improved comparison of Gaussian vs Lorentzian lineshapes.

Page 17 – Reworded paragraph on truncation artefacts.

Page 18 – Elaborated on Kramers-Kronig relations, and included a citation.

Page 18 – Added Footnote ††† to mention the lock's use of dispersion lineshapes for monitoring field drifts.

Page 22 – Removed footnote discussing consideration of linewidth for T_2 measurement, as this is not reliable.

Page 26 – Ralph commented that iterative methods are employed routinely in ^{13}C NMR for metabolomics fingerprinting. I am unaware of this; from what I am aware, the typical method of performing metabolomics fingerprinting is to break up spectrum into small regions (bins), integrate these bins, and then input the integrals into some routine for multivariate analysis, such as PCA. I have added the phrase "like VARPRO and AMARES" to clarify what I mean by an "iterative method".

Page 27 – Improved wording of why holistically analysing a 2D dataset can be better than sequentially analysing 1D increments.

Page 31 – Added citations to make the fact that the routine makes use of previous theory more explicit.

Page 32 – Peter mentioned that a square root was absent in the probability density (what was Equation 2.3 in my pre-viva draft). The square root wasn't present as the expression was the product of the PDFs of the real and imaginary components of a particular datapoint. I have rewritten this to make the origin of the scaling factor more clear.

Page 34 – Added Footnote † to give the definition of a matrix pencil.

Page 66 – Mentioned that the filtering process could likely be replaced by the simpler method of using a rectangular filter and slicing at the filter boundaries.

Page 71 – Figure 3.1: Replaced landscape figure with portrait version. Included a description of the different peak colours in the caption.

Page 74 – Figure 3.2: Replaced landscape figure with portrait version. Added structure of andrographolide.

Page 77 – Figure 3.3: Added structure of cyclosporin, and edited the caption accordingly.

Page 79 – Replaced "the spin tumbles" with "the molecule that the spin is associated with tumbles".

Page 83 – $T_1 \ll T_2 \rightarrow T_1 \gg T_2$.

Page 83 – Fixed unit of constant c in Stejskal-Tanner.

Page 82 – Figure 3.4: Tweaked the relative widths of pulses and gradients.

Page 90 – Mentioned that the errors for D, T_1, T_2 measurements can be obtained using the Hessian at convergence in the main text. An explicit derivation of the expression for errors is provided in the appendix.

Page 91 – Figure 3.5: Edited panel d; changed the aspect ratio and viewing angle. Hopefully the lineshapes look better with the altered view. If you still think it looks odd, I could simply remove the panel altogether; it is not the most crucial aspect of the figure.

Page 92 – Figure 3.6: Replaced landscape figure with portrait version. Added structure of andrographolide.

Page 94 – Figure 3.7: Added structures of valine, threonine and major anomeric forms of glucose.

Page 118 – Figure 4.6: Added structure of strychnine.

Page 120 – Figure 4.7: Added structure of quinine.

Page 122 – Figure 4.8: Added structure of camphor.

Page 123 – Figure 4.9: Replaced landscape figure with portrait version. Added structure of dexamethaone.

Page 125 – Figure 4.10: Added structure of estradiol.