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 $\tilde{\boldsymbol{i}}$ and $\tilde{\boldsymbol{j}}$.

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 11 – "is sent to" → "travels to".

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

Page 12 – 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 25 – 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 69 – Figure 3.1: Replaced landscape figure with portrait version. Included a description of the different peak colours in the caption.

Page 72 – Figure 3.2: Replaced landscape figure with portrait version. Added structure of andrographolide.

Page 75 – Figure 3.3: Added structure of cyclosporin, and edited the caption accordingly.

Page 80 – Figure 3.4: Tweaked the relative widths of pulses and gradients.

Page 89 – Figure 3.5: Edited panel d; changed the aspect ratio and viewing angle.

Page 90 – Figure 3.6: Replaced landscape figure with portrait version. Added structure of andrographolide.

Page 92 – Figure 3.7: Added structures of valine, threonine and major anomeric forms of glucose.

Page 116 – Figure 4.6: Added structure of strychnine.

Page 118 – Figure 4.7: Added structure of quinine.

Page 120 – Figure 4.8: Added structure of camphor.

Page 121 – Figure 4.9: Replaced landscape figure with portrait version. Added structure of dexamethaone.

Page 123 – Figure 4.10: Added structure of estradiol.