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4 NMR ANALYSIS OF HEXYLAMINE

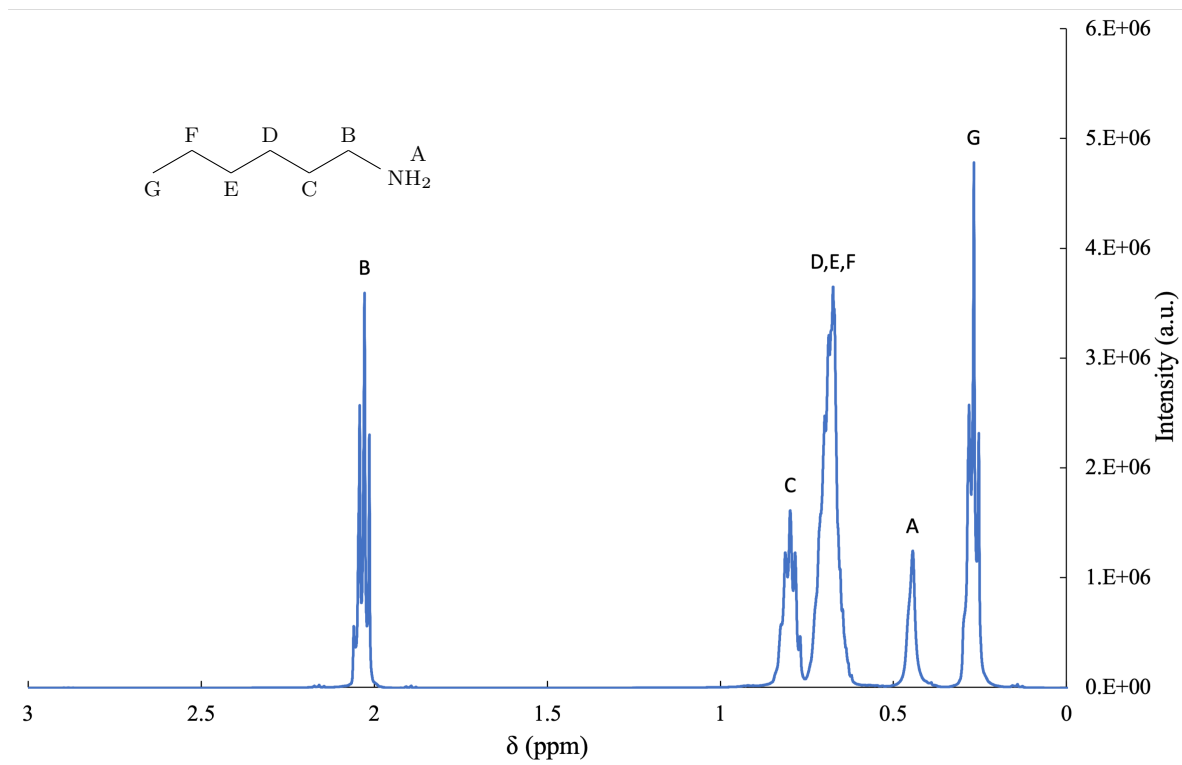


Figure 1: ^1H NMR spectrum of hexylamine. The protons on nitrogen exchange rapidly in solution, so since chemical exchanges cause spin decoupling, the A peak is a singlet.

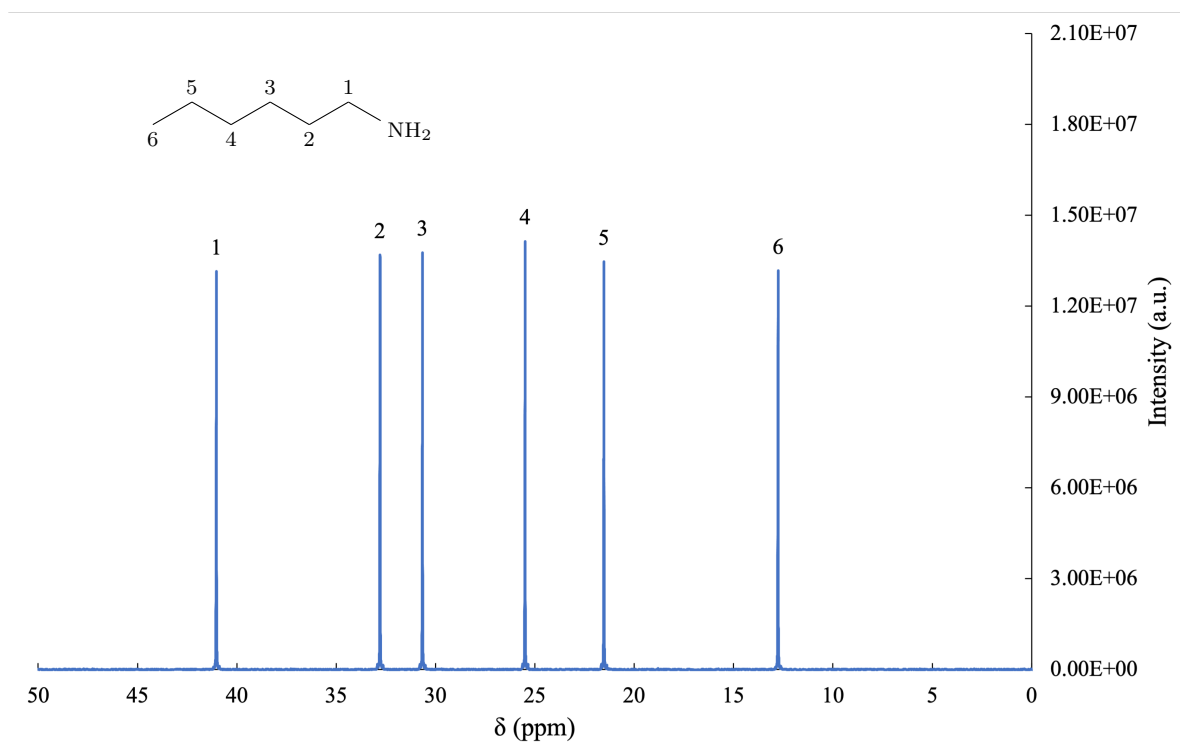


Figure 2: ^{13}C NMR spectrum of hexylamine. Notice that carbon 1 is the most downshifted because it's closest to the electronegative nitrogen atom.

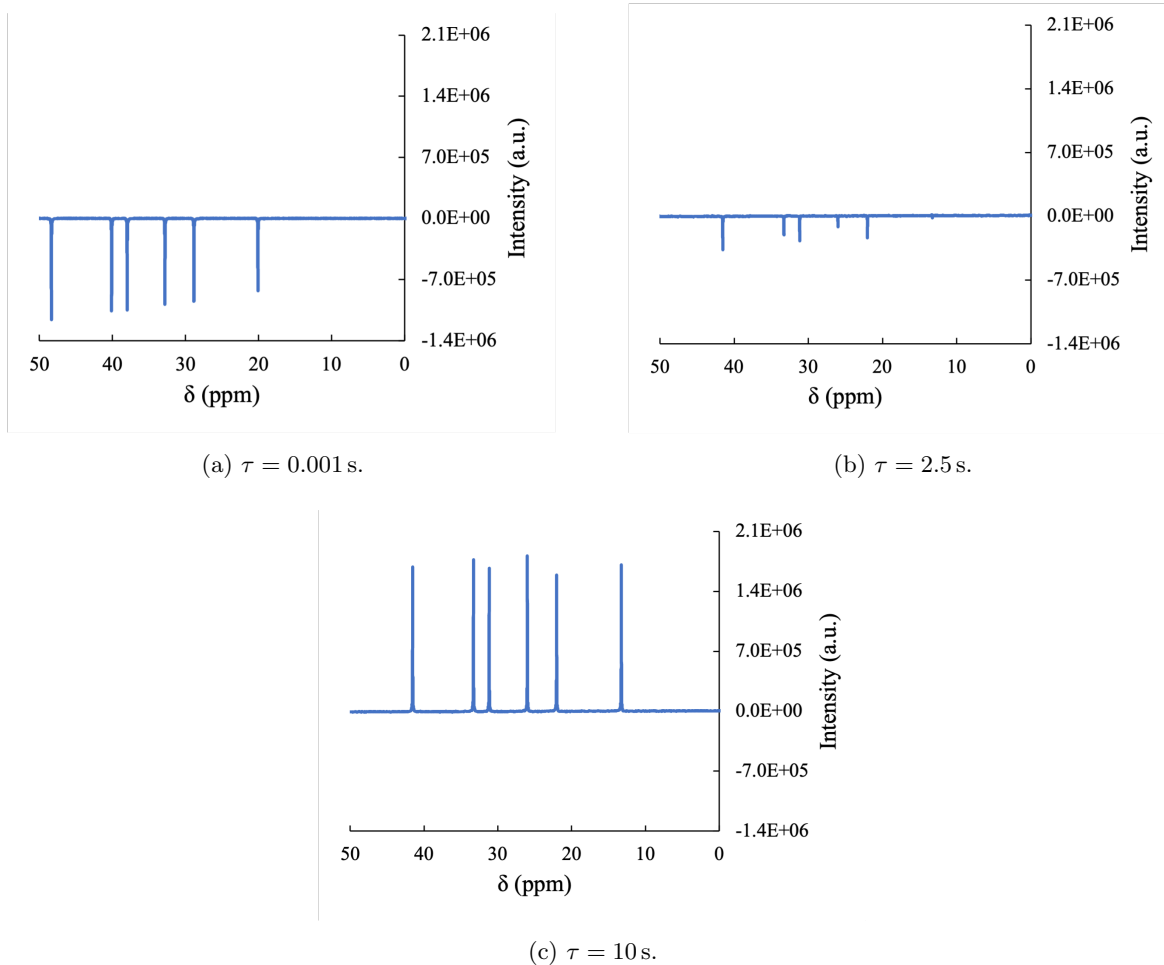
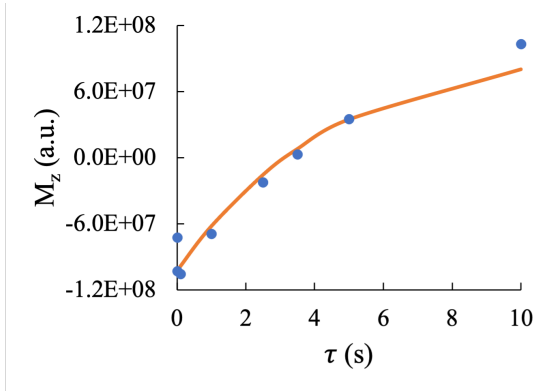
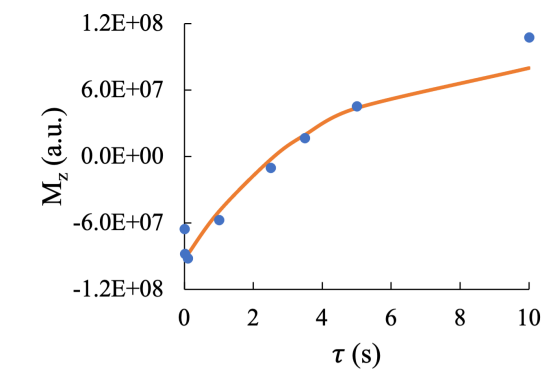


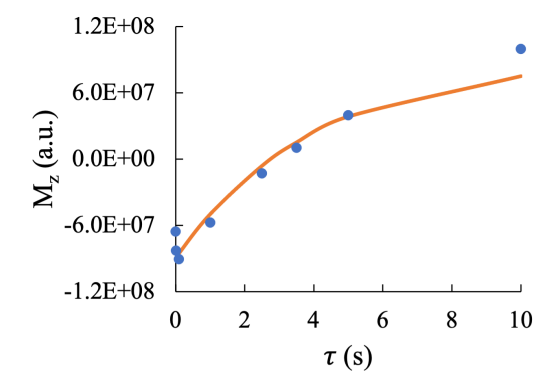
Figure 3: A selection of inversion recovery ^{13}C NMR spectra for different delay times τ .



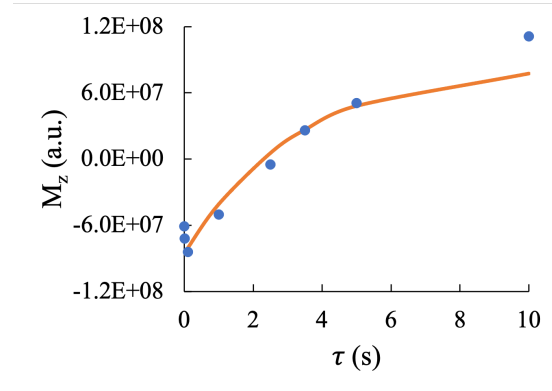
(a) Carbon 1.



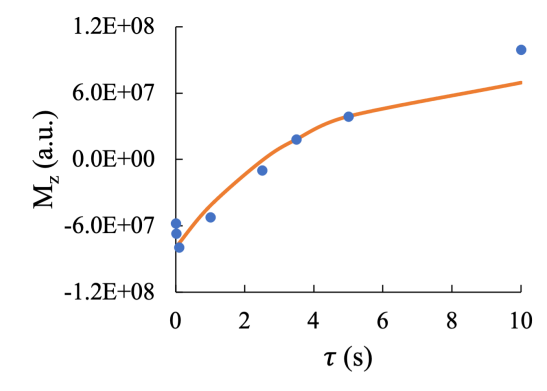
(b) Carbon 2.



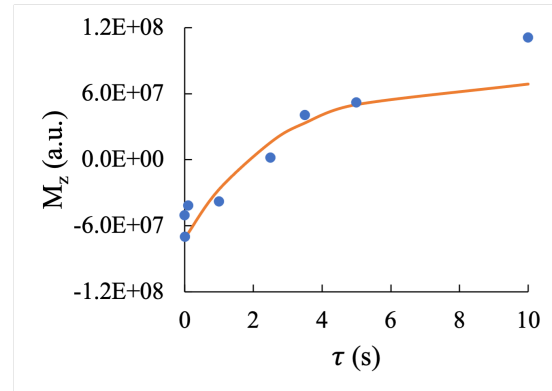
(c) Carbon 3.



(d) Carbon 4.



(e) Carbon 5.



(f) Carbon 6.

Figure 4: Determining the spin-lattice relaxation time T_1 and the magnetization M_0 at equilibrium via nonlinear regression.

Carbon 1	Carbon 2	Carbon 3	Carbon 4	Carbon 5	Carbon 6
15 197 494.17	15 490 978.25	14 146 608.68	17 608 862.89	15 739 108.37	21 625 158.79

Table 1: Standard errors for the above nonlinear regressions.

	Carbon 1	Carbon 2	Carbon 3	Carbon 4	Carbon 5	Carbon 6
T_1 (s)	4.52	3.75	3.99	3.29	3.67	2.66
τ_C (ps/rad)	5.15	6.21	5.83	7.07	6.34	5.83

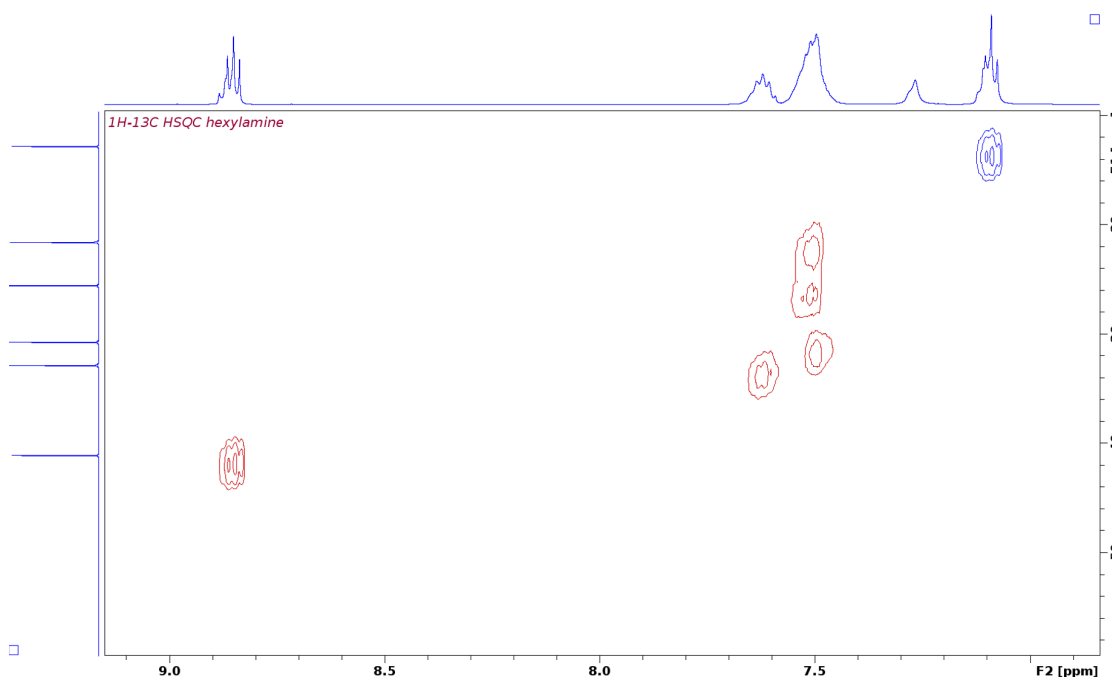
Table 2: The spin-lattice relaxation time and correlation time for each carbon in hexylamine.

Note that to calculate τ_C from T_1 , the formula

$$\frac{1}{T_1} = n \left(\frac{\mu_0}{4\pi} \right)^2 \frac{\hbar^2 \gamma_C^2 \gamma_H^2}{r_{CH}^6} \tau_C$$

was used, where the values of γ_C and γ_H were obtained from **bib:C13H1gyroempty citation** and the value of r_{CH} was obtained from **bib:CRCHandbookempty citation**.

T_1 is the time constant governing how quickly magnetic spins return to equilibrium after a disturbance. The data in Table 2 shows that T_1 trends downward for carbon atoms progressively farther from the amine moiety. This implies that carbons farther from the NH_2 group return to equilibrium more quickly. This would support a theory that the hydrogen-bonding interactions present at the NH_2 group restrict freedom in this molecule, and that portions of it farther from the center of restriction can move more freely and equilibrate more quickly. Since τ_C is related to freedom of motion directly (it is literally a measure of the time required to change angle), the above commentary also applies to it.

Figure 5: Two-dimensional ^1H - ^{13}C HSQC spectrum of hexylamine.

The peaks at the top of the HSQC spectrum in Figure 5 are analogous to those in the ^1H spectrum of hexylamine. Similarly, those on the left side of the above image are analogous to those in the ^{13}C spectrum of hexylamine. HSQC transfers magnetism between bound protons and ^{13}C atoms, so moieties that resonate in both forms of spectroscopy show up as two-dimensional peaks; in other words, each 2D peak corresponds to the proton above it and the carbon to the left of it. Thus, the six distinct peaks in the 2D spectrum correspond to the six carbons and their associated protons. The one hydrogen peak with no corresponding carbon peak represents the protons on the NH_2 moiety, providing additional evidence for the identification of that peak beyond the fact that it's a singlet per rapid proton transfer-induced spin decoupling.