# BCMB/CHEM 8190 MIDTERM
## Answers. 3/5/04

Part I.

1 a) $(15-4.8)\times 600\times 2 \approx 12{,}250$ Hz

b) $(16-4.8)\times 600 = 6720$, $\frac{12{,}250}{2} - 6720 =$ 595 Hz. (11655 also OK)

2. poor S/N - function attenuates $t=0$ part of FID strongly.

3. $\theta = 90$

4. Puke imperfections can be viewed as $\theta = 90 + \Delta \cdot 90$
Look at $I_z$ coefficient & expand in series. $\approx 1-2\Delta^2$ in first. $\approx 1-2\Delta^4$ in second when $\Delta$ is $<<1$. error in second is smaller.

Part II.

1. 360° requires $\frac{1}{1000}$ s.
   in $1 \times 10^{-4}$ s, 36° error

2. $LW = \frac{1}{\pi T_2} = 15.9\ Hz$

3. $\frac{I_1}{I_2} = \frac{0.3}{1.0} = \left(\frac{r_2}{r_1}\right)^6 = \left(\frac{r_2}{3.5}\right)^6$

   $r_2 = 2.86$

4. HSQC. starts with $^2H$ mag & detects $^2H$ mag. $\therefore$ $(\gamma_H/\gamma_D)^3$ advantage per scan is 64. to get quadrature in indirect dimension. need $2 \times 64$ scans. $\therefore$ HSQC would take 2x as long. or hav. $\frac{1}{\sqrt{2}}$ less sensitivity for equal time.

# Part III

a) neglect $S_z$ at eq. for a low $\gamma$ nucleus.

$$I_z \xrightarrow{90x} -I_y \xrightarrow{J/2} 2I_xS_z \xrightarrow{90x} -2I_xS_y$$

$$I_z \xrightarrow{90y} I_x \xrightarrow{J/2} 2I_yS_z \xrightarrow{90x} 2I_yS_x$$

b) $2I_yS_x - 2I_xS_y = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$\alpha\beta \rightarrow \beta\alpha$ transitions are populated.
this is zero quantum coherence.

c) $\xrightarrow{180x}$ $-2I_xS_y$
$\xrightarrow{180x}$ $-2I_yS_x$
matricies now add.

$$= \begin{bmatrix} 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

this is two quant. coherence.

net effect: $^1H$ evolution cancels. only $S_z$ evolves.

Part 4

a) $H_2$ - 5.05, $H_3$ - 5.26, $H_4$ - 3.86
$H_5$ - 3.77

b). one can see from the multiplet at 3.77 that the $H_5$-$H_6$ couplings are small + TOCSY Transfers inefficient. also. this is the last transfer in a long chain.

c) there is second orcler coupling to the peaks at 5.12. Yes the couplings can be measured.- A-B Type second order effects don't change couplings. The smaller couplings are 1st order.