

**BCMB 8190**  
**ANSWERS TO PROBLEM SET 6**

1)

a)  $2I_x S_z \xrightarrow{I_y + I_y} -2I_z S_x$

b)  $\tilde{I}_z S_x = \frac{1}{4} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$



2)

$$I_{z^2} + S_z \xrightarrow{\frac{I_x}{\hbar}} -I_y + S_z \xrightarrow[\tau = \frac{\hbar}{2J}]{J I_z S_z} \quad (180^\circ)$$

$$\rightarrow -2 I_x S_z + S_z$$

$$\begin{array}{l} I_x (\frac{\hbar}{2}) \\ \xrightarrow{\quad} \\ S_y (\frac{\hbar}{2}) \end{array} \begin{array}{l} -2 I_x S_x + S_x \\ \xrightarrow{\quad} \\ \end{array} \begin{array}{l} \hat{H}_1 \\ \xrightarrow{\quad} \\ I_z + S_z \\ + \\ 2 I_z S_z \end{array}$$

$$\rightarrow \begin{array}{l} a_1 I_x S_x + a_2 I_y S_x + a_3 I_x S_y \\ + a_4 I_y S_y \\ a_5 I_z S_y + a_6 S_y + a_7 I_z S_x \\ + a_8 S_x \end{array}$$

$$\begin{array}{l} S_y (\frac{\hbar}{2}) \\ \xrightarrow{\quad} \end{array} \begin{array}{l} a_1 I_x S_z + \text{---} + \text{---} \\ + \text{---} \\ + \text{---} + \text{---} + \text{---} \\ + \text{---} \end{array}$$

only observable comes from  $I_x S_x$   
or  $ZQ + ZQ$  evolution in  $t_f$ .

3)

(a)

spin system 1. (approx. ppm)

5.10, 4.05, 3.85, 3.66, 3.74, 3.74, 3.86

spin system 2.

4.90, 3.98, 3.92, 3.65, 3.68, 3.74, 3.86

spin system 3

4.70, 4.08, 3.83, 3.89, 3.78, 4.00, 3.72

all 3 are pyranoses: H<sub>1</sub>, H<sub>2</sub>, H<sub>3</sub>, H<sub>4</sub>, H<sub>5</sub>, H<sub>6</sub>, H<sub>6'</sub>

Couplings.  $^3J_{12} + ^3J_{23}$  are small;  $< 5 \text{ Hz}$ .

The rest are large - This is characteristic of mannose.

H<sub>1</sub>-shifts. below 4.7 ppm  $\Rightarrow$   $\alpha$  mannose.

(b) see labels on HSQC, HMBC for assignments. Residue 1 is clearly connected to a CH<sub>3</sub> via its anomeric carbon (1). residue 2 is connected to C<sub>6</sub> of 1. residue 3 is connected to C<sub>3</sub> of 1.



