

**BCMB/CHEM 8190
PROBLEM SET 6**

- 1) a) In product operator notation, show the effect of a short (hits both spins) 90 degree rf pulse about the + y axis on the density matrix represented by the I_1xI_2z product operator.
- b) Show the density matrix equivalent (fill in elements of matrix) of the result in a two spin 1/2 system and sketch the spectrum that would result from observing x magnetization.

- 2) Using product operators for a pair of spin 1/2 nuclei, identify the operators evolving during t_1 that are detectable during t_2 as I spin magnetization. The two spins are scalar coupled with value J and t is set to $1/(2J)$.

I---90x--t/2--180x--t/2--90x----- Acquire

S-----180x-----90y-----t1-----90y---t2---

- 3) The following three images show COSY, TOCSY, HSQC, and HMBC spectra for a methyl glycoside of a trisaccharide composed of three identical pyranose moieties (courtesy of Eric Sayers). Please note that the scales are not the same in all spectra, and only portions of the spectra are shown.

a) Using the COSY and TOCSY spectra try to trace out the 7 proton spins in each spin system. Based on the size of couplings and intensities of crosspeaks, what is the monosaccharide involved?

b) Using the HSQC and the HMBC spectra identify the linkage sites. What is the structure of the molecule? Remember that in the HMBC the primary transfers seen are 3 bond transfers. Couplings for both 2 bond and 4 bond pairs are small.





