

BCMB/CHEM 8190

PROBLEM SET 5

1) If you try to measure a scalar coupling from the splitting of the two most downfield lines in an AB spectrum, will the value you measure be equal to, larger than, or smaller than the true coupling? Will the chemical shift you try to measure from the center of the two lines be equal to, more downfield, or more up field than the true chemical shift?

2) Derive a matrix representation for the I_x operator using the eigenfunctions for a spin 1 nucleus in a static magnetic field as a basis set. Use matrix methods to find the relative intensities of $1 - 0$ and $1 - -1$ transitions associated with this operator. You will find the general expression for the effect of raising and lowering operators on spin functions useful in doing this: $I(+)(\psi(l,m)) = ((l(l+1)-m(m+1))^{1/2}) (\psi(l,m+1))$, $I(-)(\psi(l,m)) = ((l(l+1)-m(m-1))^{1/2}) (\psi(l,m-1))$.

3) Use density matrix methods to examine magnetization for a pair of spin 1/2 nuclei in a magnetic field B_0 along the z axis.

a). Show the elements of an equilibrium density matrix (σ) in the simple product basis set basis set.

b). Calculate equilibrium z magnetization using matrix methods.

c). Find the frequency at which the 1,2 element oscillates.

d). At what frequency does the 1, 4 element oscillate?