| HW 5            | Multinuclear NMR | Name:     |  |
|-----------------|------------------|-----------|--|
| Points:         | C6800            | Date:     |  |
| Max. 100 points | Spring 2011      | Version A |  |

1. Derive an expression for pH value as a function of observed chemical shift in a weak acid BH<sup>+</sup> system, when pK<sub>a</sub> is known and  $\delta_B$ ,  $\delta_{BH}$  were measured independently:

 $BH^+ \leftrightarrow B + H^+$ 

$$pH = f(\delta_{obs}, \delta_B, \delta_{BH}, pK_a)$$

$$K_{a} = \frac{[H][B]}{[HB]} \qquad \qquad \delta_{obs} = \frac{\delta_{B}[B] + \delta_{BH}[BH]}{[B] + [BH]}$$