CH3F5 Quantifying Molecular Interactions - Examples Class

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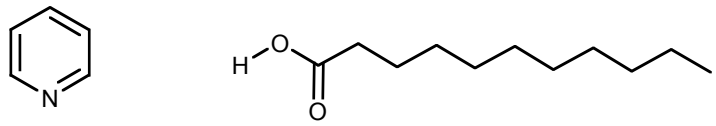
1. Estimate the change in free energy upon association, $\Delta\Delta G$ of molecules **1** and **2** at 298 K in:

(a) chloroform $\alpha = 2.2$, $\beta = 0.8$
(b) DMSO, $\alpha = 0.8$, $\beta = 8.9$

You will need the following data:

Pyridine $\alpha = 1.4$, $\beta = 7.0$
(Carboxylic acid) $\alpha = 3.6$, $\beta = 5.3$
R = 0.008314 kJ K^{-1} mol^{-1}



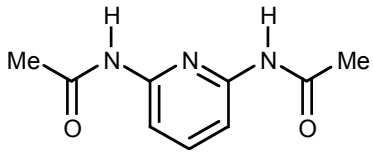
1 **2**

What is the expected association constant, K_a in each case?

2. Estimate the change in free energy upon association, $\Delta\Delta G$ of molecules **3** and **4** at 298 K in

(a) chloroform $\alpha = 2.2$, $\beta = 0.8$
(b) DMSO, $\alpha = 0.8$, $\beta = 8.9$

You will need the following data:
Amide $\alpha = 2.9$, $\beta = 8.3$
Pyridyl $\alpha = 1.4$, $\beta = 7.0$
R = 0.008314 kJ K^{-1} mol^{-1}



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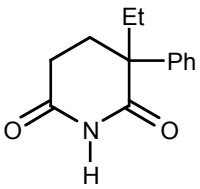

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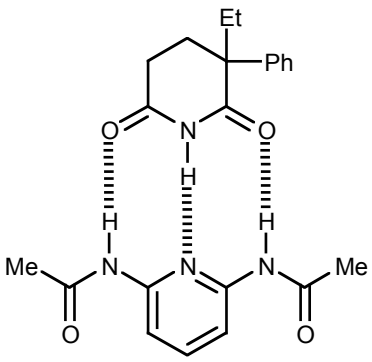

What is the expected association constant, K_a in each case?