# A Statistical Model of Hydrogen Bonding


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## 1. Introduction

Polymers and their interactions are of fundamental importance for many applications in materials sciences/technological applications including the increasing of yield or understanding how one can create 'greener' chemical processes. Hydrogen bonding is ubiquitous in nature, from holding individual water molecules to one another to the formation of the bihelical structure of DNA. This piece of work was completed as a 6 week UROS (Undergraduate Research Opportunities Scheme) project with the aim of finding how likely hydrogen bonds are to form in given systems.

## 2. Method

The method for the consideration of the permutations of the polymers and their bonds, putting the free energy of hydrogen bonding into the Flory-Huggins formulation were performed analytically. The xi parameter, the number of ways to form M1 bonds of one type to M2 bonds of another, was calculated to find this.

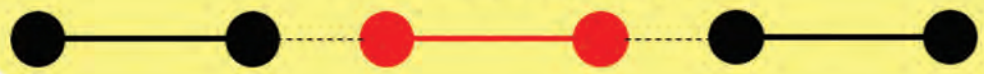
## 3. Model

There were two systems under consideration. System 1 has a self-associating polymer, A, with a donor and acceptor on either side, as well as some other polymer, B, which only has one acceptor (i.e. A-A-…-A-B). This has xi parameter:

$$\Xi = \frac{N_A!}{(N_A - M_1)!}\frac{(N_A - M_1)!}{(N_A - M_1 - M_2)!}\frac{1}{M_1!}\frac{1}{M_2!}$$

System 2 has two polymers, A and B, which are not self-associating but can associate to one another (i.e. A-B-A-B-…-A-B). This has xi parameter:

$$\Xi = \frac{2N_A!}{(2N_A - M)!}\frac{2N_B!}{(2N_B - M)!}\frac{1}{M!}$$



## 4. Flory-Huggins Formulation

A theory of mixing polymer solutions with regard to regular solution theory has been considered, this is added to the Flory-Huggins theory.

For model 1, one acquires:

$$\frac{F_{HB}}{kTV} = (m_1 + m_2)(1 + \log \phi_{A0}\phi_{B0}) + \phi_A(1 - \log \phi_A)$$

For model 2, this can be expressed as:

$$\frac{F_{HB}}{kTV} = m + 2\phi_A\left(\log\frac{2\phi_A - m}{2\phi_A} - 1\right) + 2\phi_B\left(\log\frac{2\phi_B - m}{2\phi_B} - 1\right)$$

## 5. Associativity Constants

These constants state how likely association of the polymers is to occur Model 1 has 2 parameters given by:

$$K_1 = \frac{m_1}{c_A - m_1 - m_2}; K_2 = \frac{m_2}{c_A - m_1 - m_2}$$

Model 2 has the 1 parameter:

$$K = \frac{m}{(2c_A - m)(2c_B - m)}$$

## 6. Conclusions & Future Work

In conclusion, it has been found that the two models have the xi, Flory-Huggins, and associativity parameters shown and can be calculated via combinatoric methods. The calculation of the integer sequence corresponding to α still needs to be completed for the two models. This project could be extended by performing calculations for more systems.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