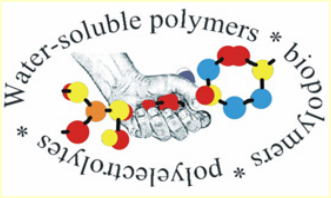

ADAPTATIVE CHEMISTRY. 3. BAYESIAN APPROACH TO DYNAMER ADAPTATION ABILITY

G. S. Georgiev

University of Sofia, Faculty of Chemistry,
Laboratory of Water-Soluble Polymers, Polyelectrolytes and Biopolymers,
1 James Bourchier Avenue, 1164-Sofia, Bulgaria

E-mail: georgs@chem.uni-sofia.bg

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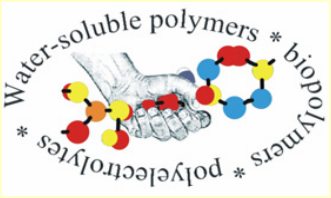

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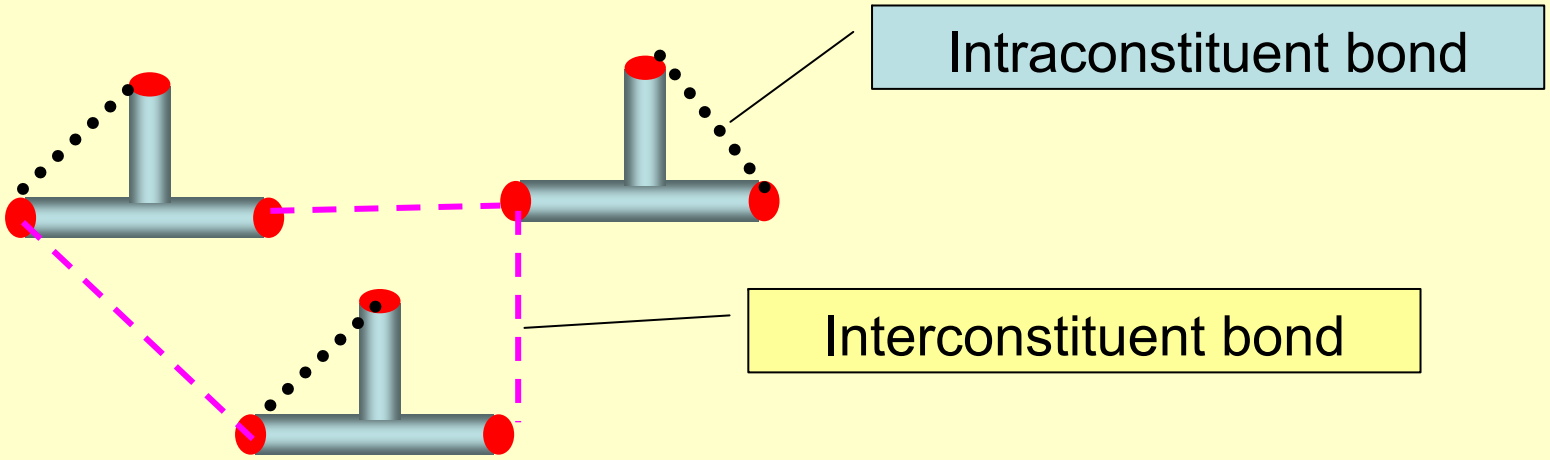
1. TWO TYPES OF ADAPTATION ABILITIES (AA): CONSTITUENT'S AND DYNAMER'S ONES



$$A_i = N_{i,r} / N_i \,, \qquad (1)$$

where A_i is the constitutional AA, N_i is the total number of the constituonal active centres, and N_{ir} is the number of the constituonal active centres occupied in the interconstituent bonds.

$$A_{ij} = (N_{i,r} + N_{j,r})/ (N_i + N_j), \qquad (2)$$

where A_{ij} is the dynamer (mutual for i and j constituents) AA.

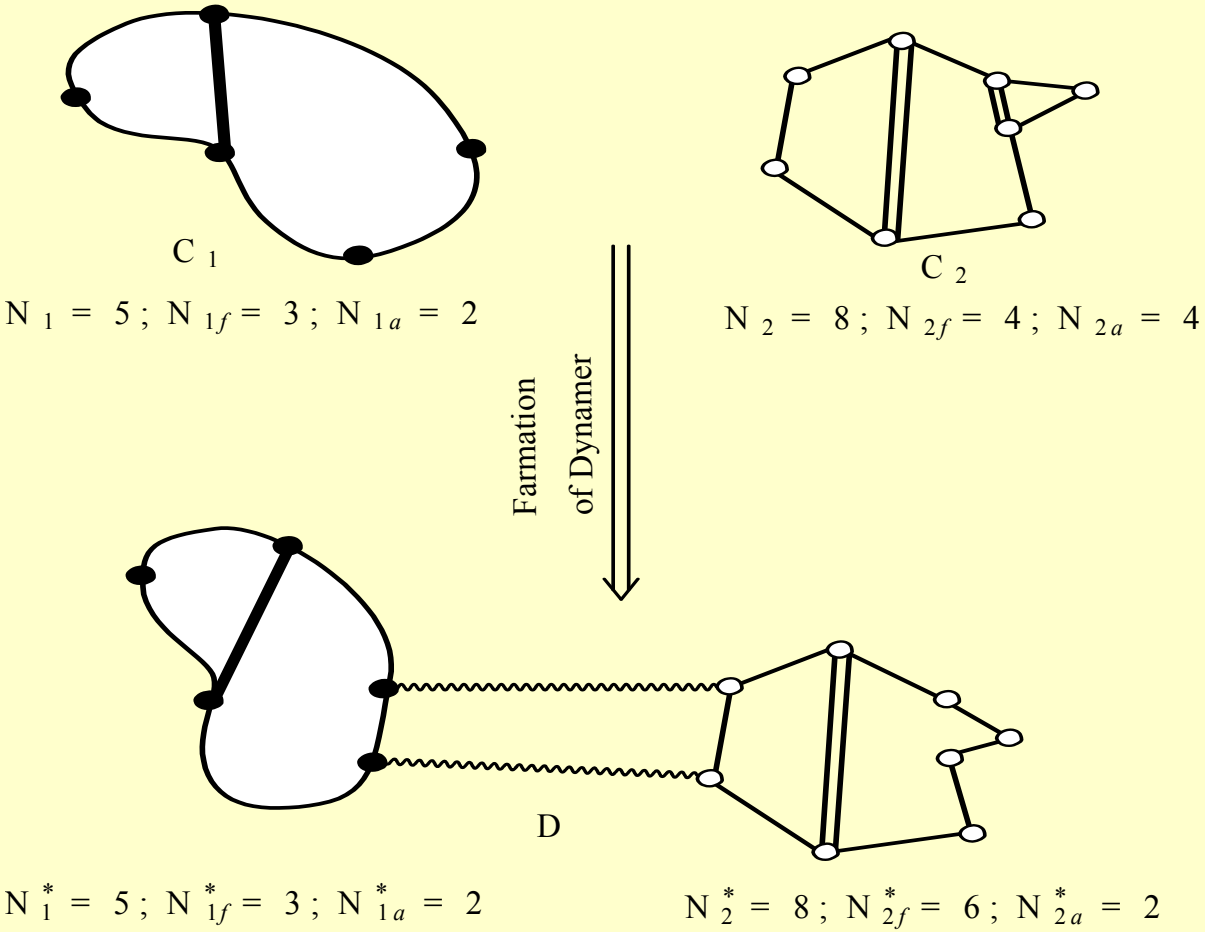
The relationship between the constituonal (A_i) and dynamer (A_{ik}) AA is deduced:

$$A_{ik} = n_i A_i + N_k A_k , \qquad (3)$$

where n_i and n_k are the number fractions of the i-st and k-st active centres

$$n_i = N_i / (N_i + N_k) \qquad (4)$$

2. BAYESIAN APPROACH AND CONDITIONAL PROBABILITIES FOR THE INTERCONSTITUIONAI JUNCTIONS THROUGH FREE AND OCCUPIED IN THE INTRACONSTITUENT JUNCTIONS CONSTITUENT ACTIVE CENTRES



Denotations:

- P(1), P(2) etc. – the probabilities for the interbond formation with the active centres from 1-st, 2-nd etc. constituents.
- $P_r(f/1)$ – the conditional probability for the interbond (r) formation using the free active centre of the constituent 1. Similarly, $P_r(f/2)$ could also be defined.
- $P_r(a/1)$ and $P_r(a/1)$ – the conditional probabilities for the interbond formation using the active centres of both constituents (1 and 2) occupied for the formation of the intraconstituent bonds.

$$P(1) = N_1/(N_1 + N_2) \quad (5)$$

$$P(2) = N_2/(N_1 + N_2) \quad (6)$$

$$P_r(f/1) = (N_{1,f} - N^*_{1,f})/N_1 \quad (7)$$

$$P_r(f/2) = (N_{2,f} - N^*_{2,f})/N_2 \quad (8)$$

$$P_r(a/1) = (N_{1,a} - N^*_{1,a})/N_1 \quad (9)$$

$$P_r(a/2) = (N_{2,a} - N^*_{2,a})/ N_2 \quad (10)$$

According to the Bayesian theorem the relations of the probability for the interbond formation using free active centres of the constituents 1 and 2 were deduced:

$$Pr(1/f) = Pr(f/1)P(1) / (Pr(f/1)P(1) + Pr(f/2)P(2)$$
$$= (N1,f-N^*1,f) / (N1,f + N2,f) – (N^*1,f + N^*2,f)) \quad (11)$$

$$Pr(2/f) = Pr(f/2)P(2) / (Pr(f/1)P(1) + Pr(f/2)P(2)$$
$$= (N2,f-N^*2,f) / (N1,f + N2,f) – (N^*1,f + N^*2,f)) \quad (12)$$

By the same way the similar relations were deduced for the probabilities for the interbond formation using the occupied in the intraconstituent bonds active centres (Pr(1/a) and Pr (2/a)).

Relationships were also deduced between the adaptation abilities, mentioned above and these Bayesian probabilities:

$$Pr(i/a) = A^a_i / A^a_{ij} \quad (13)$$

$$Pr(i/f) = A^f_i / A^f_{ij} \quad (14)$$

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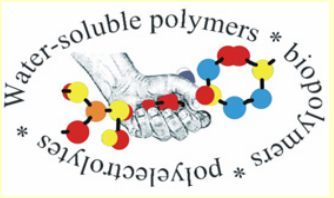

THANKS FOR YOUR ATTENTION!