A Soap Bubble Model for Coalescence, Rearrangement, and Splitting Reactions of Fullerenes

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Synopsis. Coalescence, rearrangement, and splitting reactions of fullerenes are examined by use of a soap bubble model, where fullerenes are replaced by soap bubbles of a perfectly elastic body, to yield the predictions of the modes of these processes.

Recently, Yeretzian et al. reported coalescence reactions (Eqs. 1a and 1b) of fullerenes.[1)]

$$2C_{60} \rightarrow C_{118} + C_2. \quad (1a)$$

$$2C_{70} \rightarrow C_{138} + C_2. \quad (1b)$$

Here fullerenes lose a small number of carbon atoms. These phenomena are examined by a soap bubble model, where a fullerene is replaced by a soap bubble of a perfectly elastic body. The total energy E of a soap bubble is given by

$$E = T + V, \quad (2)$$

where T and V are the kinetic and potential energy of a soap bubble, respectively. For a soap bubble of a perfectly elastic body, T and V must be conserved. Since a fullerene is electrically neutral, V is given by

$$V = \sigma S, \quad (3)$$

where σ is the surface tension and S the area of a soap bubble surface. Thus, the area of a fullerene molecular surface have to be conserved throughout the reaction. We assume that the surface tension does not depend on the size of a soap bubble.

Coalescence

Let us consider a coalescence of fullerenes of the form

$$A + B \rightarrow C. \quad (4)$$

The difference in the area of the fullerene molecular surface between the final and initial states is defined as

$$\Delta S \equiv S_C - (S_A + S_B), \quad (5)$$

where S_A (S_B, S_C) is the surface area of fullerene A (B, C). We note that the area of a fullerene molecular surface is given by

$$S = \left(\frac{N}{2} - 10\right) \cdot s_6 + 12 s_5, \quad (6)$$

where s_5 (s_6) is the area of a pentagon (hexagon) on a fullerene molecular surface, N is the number of carbon atoms constituting a fullerene molecule. Substituting Eq. 6 into Eq. 5, we obtain

$$\Delta S = \left(\frac{N_C - N_A - N_B}{2} + 10\right) \cdot s_6 - 12 s_5. \quad (7)$$

Since the area of the fullerene molecular surface have to be conserved ($\Delta S = 0$), we find

$$N_C = N_A + N_B - 20 + 24\frac{s_5}{s_6}. \quad (8)$$

This equation allows as to predict the mode of coalescence reactions of fullerenes. The results are summarized in Table 1.

For C_{60} and C_{70}, s_5/s_6 is ca. 0.76.[2)] As seen in Table 1, reaction mode I is probable for coalescence of fullerenes, in agreement with the observation.[1)] This model can be useful in studying coalescence of fullerenes accompanying the loss of carbon atoms.

Rearrangement and Splitting

We then apply the above model to rearrangement and splitting reactions of fullerenes, represented by Eqs. 9 and 10.

$$A + B \rightarrow C + D. \quad (9)$$

$$A \rightarrow B + C. \quad (10)$$

Table 1. Predicted Modes of Coalescence Reactions of Fullerenes[a)]

s_5/s_6	Mode[b)]		
	I	II	III
$<5/6$	○		
$=5/6$		○	
$>5/6$			○

a) ○, favorable; blank, unfavorable. b) Modes I, II, and III are cases where the number of carbon atoms are decreased, conserved, and increased, respectively.

Table 2. Predicted Modes of Rearrangement and Splitting Reactions of Fullerenes, by Assuming $s_5/s_6 = 0.76$[a)]

Reaction	Mode[b)]		
	I	II	III
Rearrangement		○	
Splitting			○

a) ○, favorable; blank, unfavorable. b) See footnote of Table 1 for modes I, II, and III.

Using Eq. 6 and $\Delta S=0$, we find the following conditions for the rearrangement and splitting of fullerenes:

$$\text{Rearrangement} : N_C + N_D = N_A + N_B. \quad (11)$$

$$\text{Splitting} : N_B + N_C = N_A + 20 - 24\frac{s_5}{s_6}. \quad (12)$$

Based on these equations, we can predict the mode of rearrangement and splitting reactions of fullerenes as summarized in Table 2.

There have been no clear examples of rearrangement and splitting reactions of fullerenes to date. To verify this model, we should examine the change in the number of carbon atoms accompanying the reactions.

References

1) C. Yeretzian, K. Hansen, F. Diederich, and P. L. Whetten, *Nature*, **359**, 44 (1992).

2) H. W. Kroto, A. W. Allaf, and S. P. Balm, *Chem. Rev.*, **91**, 1213 (1991).