

## Singlet and Triplet Molecular Interaction in Excimers

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A perturbative approach is developed to determine, term by term, the contributions of the various forces to the excimer potentials of the singlet and triplet excimers. The results show that the singlet excimer of naphthalene is more stable than the corresponding triplet excimer primarily due to large contributions of the exciton-resonance and the dispersion energy terms. The variation of the various terms with the conformations of the excimers suggests that the singlet and triplet excimers of naphthalene cannot have identical structure.

**Key words:** Singlet excimer – triplet excimer – exciton resonance – dispersion energy.

### 1. Introduction

Since the discovery of the excimer luminescence in pyrene by Forster and Kasper [1], the phenomenon of excimer luminescence in aromatic hydrocarbons has been the subject of many theoretical [2–7] and experimental works [8–10]. All these treatments primarily dealt with excimer potentials which were determined from the transition energies in excimers and the interaction potentials of the ground-state dimers. This approach however, does not provide sufficient insight into the nature, the magnitude and the relative importance of the different kinds of forces that operate when an electronically excited molecule interacts with the ground state molecule. A full perturbation approach for the treatment of excimers are thought to be complicated for large molecules and was therefore not attempted in the past. From the simple first-order perturbation theory and the transition dipole arguments, Hoytink [11] observed that an interaction in the triplet excimer is negligible compared to that in the corresponding singlet excimer. Birks [12] has therefore concluded that aromatic hydrocarbons cannot form triplet excimers.

But now there are increasing experimental evidences that aromatic hydrocarbons in its lowest triplet state can associate with the ground state to form triplet excimers [13–15]. Besides, the experiments with diaryl alkanes [16] clearly indicate that the conformation of the triplet excimer of naphthalene is significantly different from the sandwich-pair geometry favoured by the singlet excimer. The object of this paper is to develop a full perturbative approach with some approximations with a view to determining, term by term, the contributions of the various forces to the excimer potentials of the singlet and triplet excimers. This will lead to a better understanding of the molecular interaction in the excited states and reveal the origin of binding in the singlet and triplet excimers of an aromatic hydrocarbon. The other objective is to seek the reason why the singlet and its corresponding triplet excimers have significantly different equilibrium conformations.

We shall consider the singlet and triplet excimers of naphthalene. The various configurations of the dimer that are examined here are:

- (1) the symmetric sandwich or totally eclipsed conformations
- (2) the tilted configuration where the relative orientation of the two molecules is such that their long-axes are parallel and their short-axes are inclined by an angle  $\alpha$
- (3) the rotated sandwich configuration where one of the molecules is rotated around the intermolecular axis by an angle  $\theta$  keeping the two molecular planes parallel.

These structures are shown in Fig. 1.

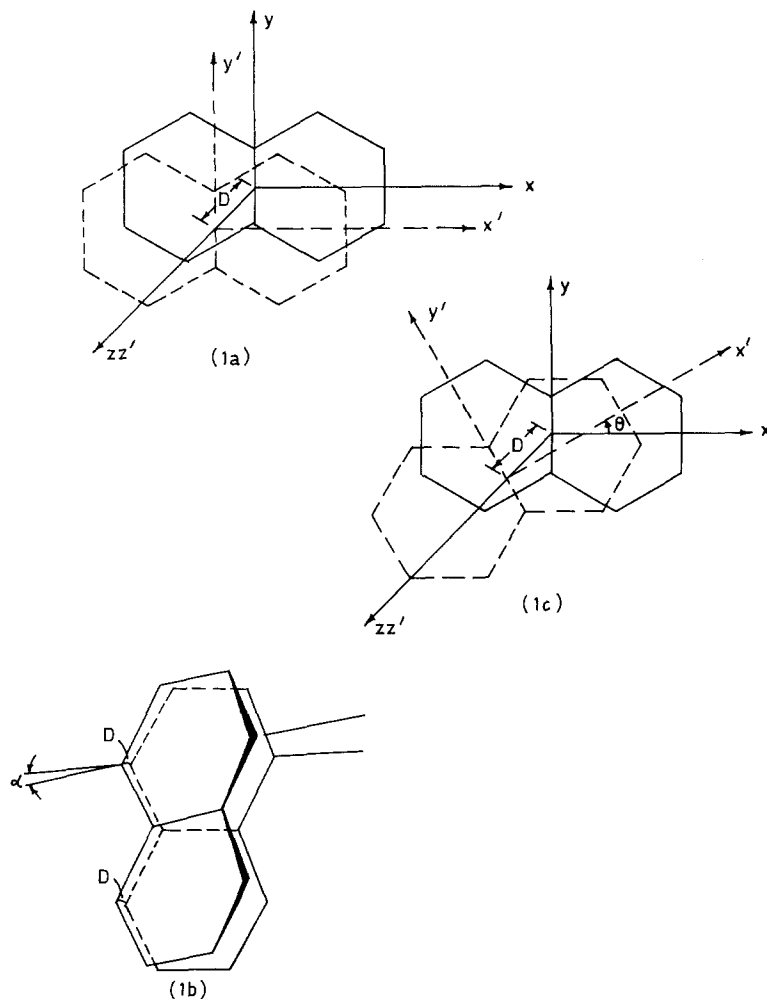
The excimer emission in naphthalene originates from the  $p$ -state (Clar notation) in monomer [17]. We therefore, assume that the singlet and the triplet excited states of naphthalene in the naphthalene excimers arise from a transition from the highest filled  $\pi$ -orbital to the lowest vacant  $\pi$ -orbital. The  $\sigma$ -core of naphthalene excimer can therefore be assumed to be the same as in the ground dimer and therefore the  $\sigma$ - $\sigma$  interaction in excimers is treated in the same manner as in the ground dimer [18]. We ignore the  $\sigma$ - $\pi$  interaction as they make very small contribution to the excimer potentials [6] and deal with the  $\sigma$ - and  $\pi$ -electrons interaction terms separately in excimers. The  $\pi$ -electron interaction terms are treated according to the following perturbation scheme.

## 2. Perturbation Theory for the $\pi$ -Electron Interaction Terms in the Excited States

Consider an interaction between two identical molecules A and B. The Hamiltonian of the composite system is

$$H = H_A + H_B + V \quad (1)$$

where  $V$  is the interaction operator. When one of these molecules is excited, the



**Fig. 1.** Axes-system for a pair of naphthalene molecules for three different steric conformations where  $D$ ,  $\alpha$  and  $\theta$  are defined

zeroth-order wave function of the composite system is given by

$$[\Psi_0]_{\pm} = \mathcal{A}[\Phi_0]_{\pm} = \frac{\mathcal{A}}{\sqrt{2}} [\psi_{A0}\psi_{B1} \pm \phi_{A1}\phi_{B0}] \quad (2)$$

where  $\mathcal{A}$  is the antisymmetriser,  $\phi_{A0}$ ,  $\phi_{A1}$  etc. represent the ground and  $p$ -state wave-functions of  $A$  (i.e. naphthalene). The electronic coordinates are so defined that the wave-function  $(\Psi_0)_-$  corresponds to the lowest excited zeroth-order state of the excimer. The other excited states of the composite system can be described by

$$\mathcal{A}[\Phi_k]_{\pm} = \frac{\mathcal{A}}{\sqrt{2}} [\phi_{As}\phi_{Bt} \pm \phi_{At}\phi_{Bs}] \quad (3)$$

where  $\phi_{B_t}$ ,  $\phi_{B_s}$  are the  $t$ th and  $s$ th excited states of  $B$ . In the perturbation scheme developed by Murrell and Shaw [19] and later by Musher and Amos [20] the perturbed wave-function of the composite system is expanded as

$$\Psi = \Psi_0 + \sum'_K C_K \Phi_K. \quad (4)$$

In Eq. (4) the + and - signs associated with the zero-order wave functions are dropped because the states of different parity do not mix and owing to the choice of the electronic coordinates, the (-)-state corresponds to the lowest energy zeroth-order state of the excimer. It should be noted that the summation in Eq. (4) includes the wave functions of the charge-transfer states which can be described by

$$[\Phi_{CT}]_{\pm} = \frac{1}{\sqrt{2}} [\phi_{A+}\phi_{B-} \pm \phi_{A-}\phi_{B+}]. \quad (5)$$

According to the MS-MA scheme [19, 20], the first-order and second order contributions to the interaction potentials of excimer are given as

$$\varepsilon^{(1)} = \frac{\langle \mathcal{A}\Phi_0 | V | \Phi_0 \rangle}{\langle \mathcal{A}\Phi_0 | \Phi_0 \rangle} \quad (6)$$

$$\varepsilon^{(2)} = \sum'_k \frac{\langle \Phi_0 | V | \Phi_K \rangle \langle \Phi_K | \mathcal{A}(V - \varepsilon^{(1)}) | \Phi_0 \rangle}{\langle \mathcal{A}\Phi_0 | \Phi_K \rangle (E_0 - E_K)}. \quad (7)$$

### 2.1. First-order interaction terms

The first-order term is obtained after substituting Eq. (2) in Eq. (6) and taking the minus combination in Eq. (2). Since  $\mathcal{A} = \mathcal{I} + \mathcal{P}$  where  $\mathcal{I}$  is the identity and  $\mathcal{P}$  the permutation operators, the first-order energy involves the three following terms.

$$\begin{aligned} \varepsilon^{(1)} = & \langle \phi_{A_0}\phi_{B_1} | V | \phi_{A_0}\phi_{B_1} \rangle \\ & + [-\langle \phi_{A_0}\phi_{B_1} | V | \phi_{A_0}\phi_{B_1} \rangle \langle \mathcal{P}\phi_{A_0}\phi_{B_1} | (\phi_{A_0}\phi_{B_1} - \phi_{A_1}\phi_{B_0}) \rangle \\ & + \langle \mathcal{P}\phi_{A_0}\phi_{B_1} | V | \phi_{A_0}\phi_{B_1} \rangle \{1 - \langle \mathcal{P}\phi_{A_0}\phi_{B_1} | (\phi_{A_0}\phi_{B_1} - \phi_{A_1}\phi_{B_0}) \rangle\} \\ & + [-\langle (\mathcal{I} + \mathcal{P})\phi_{A_0}\phi_{B_1} | V | \phi_{A_1}\phi_{B_0} \rangle \{1 - \langle \mathcal{P}\phi_{A_0}\phi_{B_1} | (\phi_{A_0}\phi_{B_1} - \phi_{A_1}\phi_{B_0}) \rangle\}]. \end{aligned} \quad (8)$$

The first two terms of Eq. (8) are respectively the electrostatic and first-order exchange energies while the third term may be called the excitation resonance energy as it originates from the delocalisation of excitation between the two component molecules.

#### 2.1.1. Electrostatic and first-order exchange energies

There should be no finite contribution of the electrostatic energy to the excimer potentials of the singlet and triplet states because an alternant hydrocarbon does not have any net  $\pi$ -electron charge on any atom in its  $p$ th electronic state. The first

order exchange energy term for the singlet and triplet excimers can be expanded, after neglecting terms which are higher than second-order in the overlap and assuming  $V$  to be an effective one-electron operator. It is given by

$$\begin{aligned}
 {}^{1,3}E_{\text{exch}}(\pi - \pi) = & -4 \sum_{i'}^{\text{occ } A} \sum_{k'}^{\text{occ } B} \langle i|v|k'\rangle \langle i|k'\rangle \\
 & - 2 \sum_i^{\text{occ } A} \langle i|V|(n+1)\rangle \langle i|(n+1)\rangle + 2 \sum_i^{\text{occ } A} \langle i|V|n'\rangle \langle i|n'\rangle
 \end{aligned} \quad (9)$$

where  $i$  and  $i'$  stand for the molecular orbitals of the molecule A and B respectively,  $n$  and  $n+1$  refer to the highest filled and lowest vacant orbitals in a monomer. The matrix elements are assumed to be proportional to the intermolecular overlap as

$$\langle i|V|j'\rangle = K_1 \langle i|j'\rangle = K_1 S_{ij'} \quad (10)$$

where  $K_1$  is a constant determined semi-empirically. Salem [21] has chosen  $K_1 = -3$  eV in the estimation of the interaction energies between two conjugated systems. We have estimated the value of  $K_1$  by fitting with the available experimental data. Birks and Kazzaz [22] have reported that the interaction energy between two ground state pyrene molecules separated by 3.34 Å in a perfect sandwich conformation is 7.9 Kcal/mole. Our calculated total interaction for this configuration of the pyrene dimer fits with the observed value for  $K_1 = -1$  eV [23]. We have adopted this value of  $K_1$  in this paper. Although this choice seems to be low, the variation of  $K_1$  in the range of  $-1$  eV to  $-3$  eV does not affect the trends of our results and our conclusions are not modified by such variations.

The first two terms of Eq. (9) are repulsive while the third term is attractive. It may be recalled that the first-term of Eq. (9) determines the first-order exchange energy (or overlap repulsion) in the ground dimer [18]. The additional terms of Eq. (9) arise from the open-shell configuration of the excimer. It should be noted that the first-order exchange energy is same for the singlet and triplet state excimer potentials, as long as the terms higher than the second-order in the overlap are ignored. Since in both the singlet and triplet excimers, the intermonomer separation is larger than 3 Å, such neglect is justified.

### 2.1.2. Exciton resonance energy

If we retain the one-electron approximation of the operator  $V$  then the exciton resonance term is same for the singlet and triplet excimers and is given by

$$\begin{aligned}
 {}^{1,3}E_{\text{ER}}(\pi - \pi) = & \langle n|V|n'\rangle \langle (n+1)|(n+1)\rangle \\
 & + \langle (n+1)|V|(n+1)\rangle \langle n|n'\rangle = 2K_1 S_{nn'} S_{(n+1),(n+1)}.
 \end{aligned} \quad (11)$$

If however, the two-electron repulsion term i.e.  $\sum_{\nu, \nu'} e^2/\gamma$  where  $\nu$  and  $\nu'$  denote the electrons of A and B respectively, is explicitly introduced in  $V$  as an after thought, it will lead to different magnitudes of the exciton-resonance energy for

the singlet and triplet excimers. Thus one obtains

$${}^{1,3}E_{ER}(\pi - \pi) = 2K_1 S_{nn'} S_{(n+1)(n+1')} - \langle n(n+1) | n'(n+1)' \rangle \pm \langle n(n+1) | n'(n+1)' \rangle \quad (12)$$

where

$$\langle ij | i'j' \rangle = \iint i(1)i'(2) \left| \frac{e^2}{\pi_{12}} \right| j(1)j'(2) dv_1 dv_2. \quad (13)$$

The negative and positive signs in the last term of Eq. (12) refer respectively to the singlet and triplet states. It is therefore immediately obvious now that the exciton-resonance stabilisation is larger in the singlet excimers than that in the corresponding triplet excimers.

## 2.2. Second-order interaction terms

The second-order interaction energy of Eq. (7) is composed of the charge-transfer, induction, dispersion and exchange energy terms. Of these, the calculation of the second-order exchange energy term is most cumbersome especially for large systems. Since it is the smallest second-order term, it can be safely ignored in the present study.

If the exchange term is ignored, then the combined charge-transfer, induction and dispersion energy terms are given by

$$\varepsilon^{(2)} = \sum_{K \neq 0} \frac{\langle \Phi_0 | V | \Phi_K \rangle \langle \Phi_K | V | \Phi_0 \rangle}{E_0 - E_K} \quad (14)$$

where the summation covers the charge-transfer states of Eq. (5) also.

### 2.2.1. Charge-transfer interaction

If in Eq. (14) the summation covers the possible charge transfer states only, arising from the transfer of an electron from any occupied orbital of *A* to any unoccupied orbital of *B* and vice versa, then the parity considerations, substitution of Eq. (2) and Eq. (5) in Eq. (14) and the expansion of wave functions in the form of the usual Slater determinants lead to Eq. (15) for the charge-transfer interaction energy.

$${}^{1,3}E_{CT}(\pi - \pi) = - \frac{[\langle n | V | n' \rangle + \langle (n+1) | V | (n+1)' \rangle]^2}{J_{n'(n+1)} - K_{n'(n+1)' \mp K_{n'(n+1)'}} - \sum_{\substack{\text{occ} \\ i \neq n}} \frac{\langle i | V | n' \rangle^2}{\varepsilon_{n'} - \varepsilon_i + J_{n'(n+1)' } - K_{n'(n+1)' \mp K_{n'(n+1)'}} - \sum_{\substack{\text{unocc} \\ i' \neq (n+1)'}} \frac{\langle (n+1) | V | i' \rangle^2}{\varepsilon_{i'} - \varepsilon_{n+1} + J_{n(n+1)} - K_{n(n+1) \mp K_{n(n+1)}}. \quad (15)$$

In Eq. (15) *J* and *K* are the usual Coulomb and exchange two-electron integrals and the  $\pm$  sign in the denominators refer to the singlet and triplet states. Eq. (15) shows that the magnitude of this term is expected to be small since, once again, it is proportional to the square of the intermolecular overlap.

### 2.2.2. Induction and Dispersion energies

Since in an alternant hydrocarbon, the static  $\pi$ -charge density on every atom is close to zero in both the ground and the  $p$ th states, the induction term is expected to be very small in an excimer and is therefore ignored. Dispersion forces however play an important role in the long-range interaction. It does not depend on the orbital overlap and is primarily determined by the polarisabilities of the component molecules. The  $\pi$ -electron polarisability of an alternant aromatic hydrocarbon is considerably large and implies a significant contribution of the  $\pi$ - $\pi$  dispersion energies to the formation of the singlet and triplet excimers. It is well known that only the two-electron interaction term can account for the dispersion interaction. It becomes therefore necessary to introduce explicitly  $\sum_{\nu,\nu'} e^2/\gamma$  in  $V$ . On substituting for  $\Phi_0$  and  $\Phi_K$  Eqs. (2) and (3) respectively into Eq. (14) and remembering that the molecules A and B are identical, one obtains

$$E_{\text{Dis}}(\pi - \pi) = -\frac{\langle \phi_{A0}\phi_{B1} | \sum_{\nu,\nu'} \frac{e^2}{\pi_{12}} |\phi_{As}\phi_{Bt}\rangle^2}{E_K - E_0} - \frac{\langle \phi_{A0}\phi_{B1} | \sum_{\nu,\nu'} \frac{e^2}{\pi_{12}} |\phi_{At}\phi_{Bs}\rangle^2}{E_K - E_0} + \frac{2\langle \phi_{A0}\phi_{B1} | \sum_{\nu,\nu'} \frac{e^2}{\pi_{12}} |\phi_{As}\phi_{Bt}\rangle \langle \phi_{At}\phi_{Bs} | \sum_{\nu,\nu'} \frac{e^2}{\pi_{12}} |\phi_{A0}\phi_{B1}\rangle}{E_K - E_0}. \quad (16)$$

In Eq. (16) we denote by subscript  $s$  all the possible singly-excited states and by  $t$  all the possible doubly excited states of the molecules A and B. If the wavefunctions on both sides of the operator  $\sum_{\nu,\nu'} e^2/\pi_{12}$  for any component molecule differs in more than one spin-orbital, the matrix element vanishes. We therefore see that the last two terms of Eq. (16) vanish. Hence, the dispersion energy for the singlet and triplet excimers is given by

$${}^{1,3}E_{\text{Dis}}(\pi - \pi) = -\sum_s \sum_t \frac{\langle \phi_{A0} {}^{1,3}\phi_{B1} | \sum_{\nu,\nu'} \frac{e^2}{\pi_{12}} | \phi_{As} {}^{1,3}\phi_{Bt} \rangle^2}{E({}^{1,3}As) + E({}^{1,3}Bt) - E({}^{1,3}A_0) - E({}^{1,3}B_1)} \quad (17)$$

where the superscripts 1 and 3 refer to the singlet and triplet state wave functions, E's denote the energies of the appropriate states indicated in the parenthesis. It should be pointed out here that the other possible triplet states i.e.  ${}^3\phi_{As}'\phi_{Bt}$  cannot make any contribution in Eq. (17) owing to the orthogonality of the spin functions. Expanding the molecular wavefunctions in the form of the Slater determinants and employing the spin-projection operator, Eq. (17) can be expanded in a workable form for the numerical computation of the dispersion energies of the singlet and triplet excimers.

### 3. Results and Discussions

Thus, the total interaction energy in a singlet and triplet excimers of an aromatic hydrocarbon is made up of the following terms:

(a) electrostatic energy ( $\sigma$ - $\sigma$ )

- |  |                   |
|--|-------------------|
| (b) overlap repulsion                  | $(\pi-\pi)$       |
| (c) exciton resonance                  | $(\pi-\pi)$       |
| (d) non-bonded repulsion               | $(\sigma-\sigma)$ |
| (e) charge-transfer interaction        | $(\pi-\pi)$       |
| (f) $\pi-\pi$ dispersion energy        |                   |
| (g) $\sigma-\sigma$ dispersion energy. |                   |

When all these terms are added we obtain the excimer potentials for the singlet and triplet states. It is to be noted that the  $\sigma-\pi$  contribution to the dispersion energy is ignored. This is partly because its calculation for excimers is cumbersome and partly because of the fact that the  $\sigma-\pi$  dispersion term does not make a serious contribution to the potentials of the ground dimers [18]. In the calculation of the  $\pi$ -electron terms we use the  $2P_{\pi}$  orbitals of the carbon atom with  $Z_c = 2.56$  as this gives the best fit to the SCF atomic function at large distances [6]. Fig. 2. shows the variation with  $D$ , the intermolecular separation, of the terms (a)–(g) and the total interaction energies of the singlet and triplet excimers of naphthalene for the symmetric sandwich geometry. As expected, the magnitude of each term

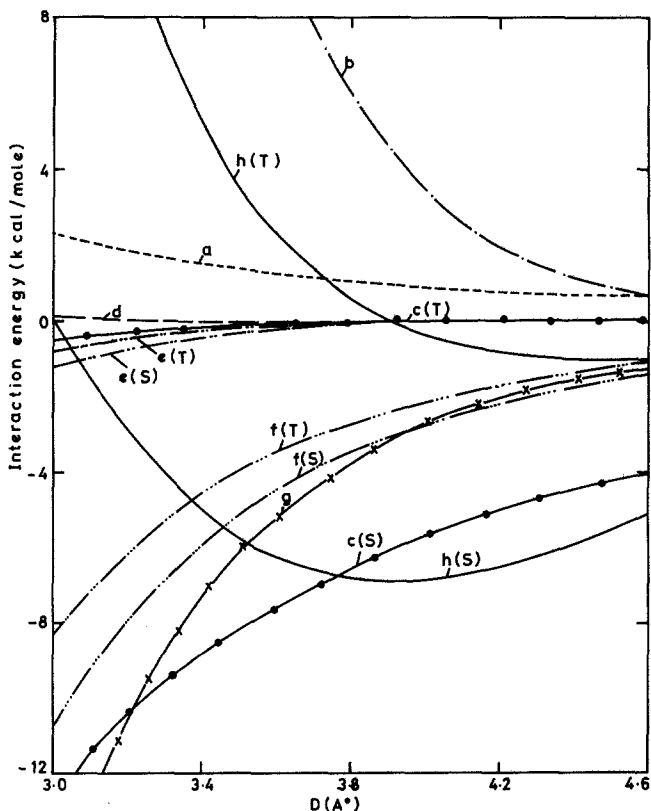
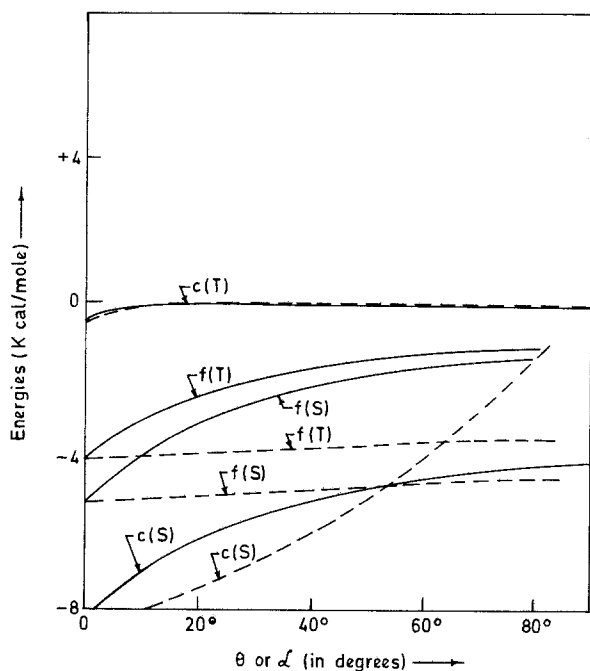


Fig. 2. Variations with  $D$  of the (a) electrostatic, (b)  $\pi$ -overlap repulsion, (c) exciton-resonance, (d) non-bonded repulsion, (e) charge-transfer interaction, (f)  $\pi-\pi$  dispersion, (g)  $\sigma-\sigma$  dispersion and (h) total interaction energy terms of the singlet (S) and triplet (T) excimers of naphthalene for the symmetric sandwich structures



decreases with the increase of  $D$ . It is seen that the magnitude of the charge-transfer term is very small in both the singlet and triplet states. Fig. 2 reveals that the main source of the stabilisation in the singlet excimer comes from the exciton-resonance, and the sum of  $\sigma$ - $\sigma$  and  $\pi$ - $\pi$  dispersion energy terms. The total dispersion term contributes more to the stability than the exciton resonance term. In the triplet excimer the contribution of the exciton-resonance is very small and hence the major attractive terms are the  $\pi$ - $\pi$  and  $\sigma$ - $\sigma$  dispersion energy terms as in the ground dimers. One therefore expects that the potentials of the triplet excimer and of the ground dimer are nearly identical.

When the exciton-resonance term is varied with  $\alpha$  and  $\theta$  for the singlet and triplet excimers, Fig. 3 shows that there is a marked decrease in the exciton-resonance term for the singlet excimer. This seems to suggest that the most stable structure of the singlet excimer of naphthalene is likely to be the perfect sandwich structure. For the triplet excimer the exciton-resonance term continues to remain very small at all values of  $\alpha$  and  $\theta$ . While the  $\pi$ - $\pi$  dispersion terms decrease gradually with  $\alpha$  in the same manner for both the singlet and triplet excimer potentials, they are almost independent of  $\theta$ . This means that the triplet excimer of naphthalene cannot have the configuration presumably favoured by the corresponding singlet excimer. In Fig. 4 and Fig. 5 are shown the variation of the total interaction energy of the singlet and triplet excimers of naphthalene with  $\alpha$  and  $\theta$  respectively for  $D$



**Fig. 3.** Variations of the (c) exciton resonance and (f)  $\pi$ - $\pi$  dispersion energy terms with  $\theta$  and  $\alpha$  for  $D = 3.5 \text{ \AA}$  in the naphthalene excimers. S and T stand for the singlet and triplet excimers. The solid and dotted lines refer respectively to the variation with  $\alpha$  and  $\theta$

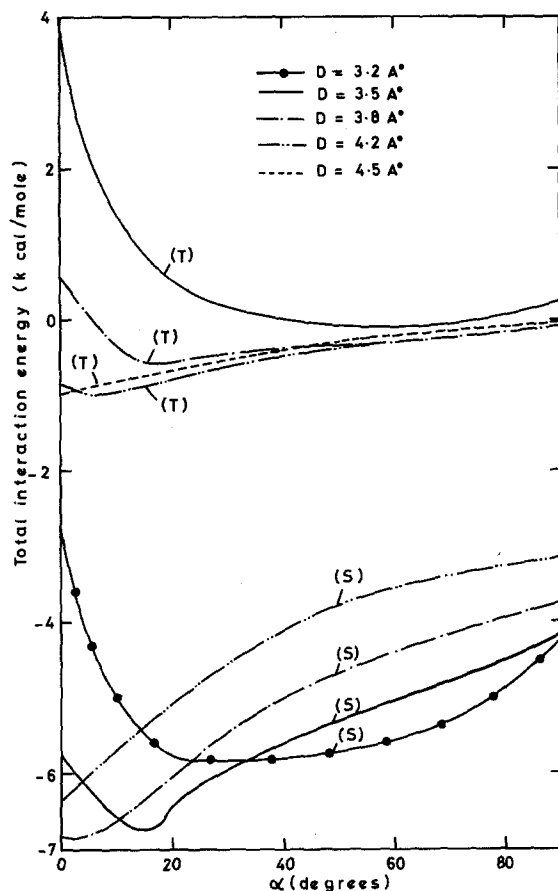
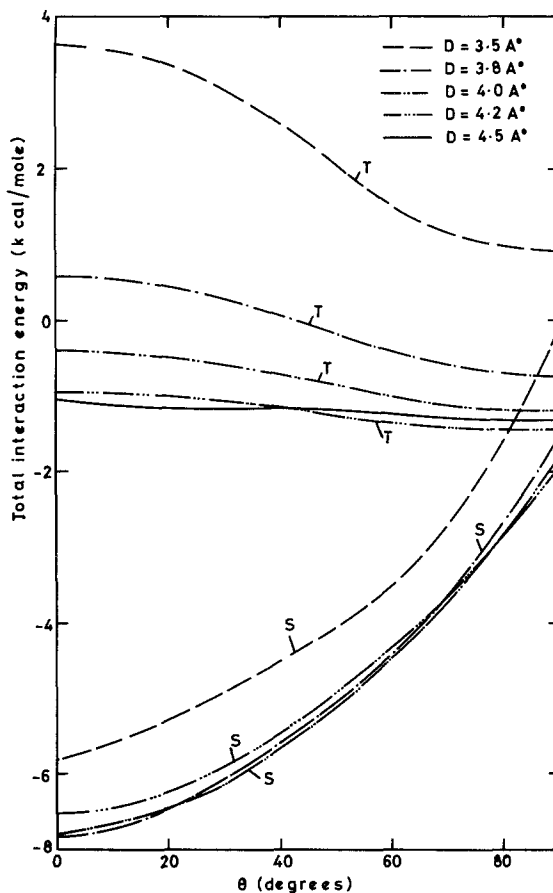


Fig. 4. Variations with  $\alpha$  of the total interaction energies in the singlet (S) and triplet (T) excimers of naphthalene at the indicated values of  $D$

in the region of  $3 \sim 4.5 \text{ \AA}$ . The results show that owing to large decrease of the exciton-resonance term the singlet excimer experiences a barrier against rotation ( $\theta$ ) and tilt ( $\alpha$ ) for  $D > 3.5 \text{ \AA}$  while the energy of the triplet excimer decreases as in the case of ground dimer. The equilibrium geometries and binding energies of the stable structures of the singlet and triplet excimers of naphthalene are obtained after minimising the total energies for different geometries. They are presented in Table 1 which shows that the calculated binding energy in the triplet excimer is less than that in the corresponding singlet excimer.

We may now conclude as follows:

- (1) The large stability of the singlet excimer is due to the exciton-resonance and the dispersion energy terms and not due to the exciton-resonance alone as was emphasised in the literatures [12].
- (2) The conformational difference between the singlet and the corresponding triplet excimers is primarily due to the exciton-resonance term.
- (3) The binding and the equilibrium conformation of the triplet excimer are controlled by the Van der Waal's forces as in the corresponding ground dimer.



**Fig. 5.** Variations with  $\theta$  of the total interaction energies in the singlet (S) and triplet (T) excimers of naphthalene at the indicated values of  $D$

**Table 1.** The possible equilibrium conformations and binding energies of the singlet and triplet excimers of naphthalene

	Singlet excimer	Triplet excimer
Conformation	Symmetric sandwich $D = 3.9 \text{ \AA}$	Rotated sandwich $D = 4.3 \text{ \AA}$ $\theta \sim 90^\circ$
Binding energy (Kcal/mole)	6.9	1.4

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