Role of the hydrogen bond in structural phototransformations of admixture centers in molecular crystals

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Structural phototransformations of admixture centers, aniline derivatives in naphthalene crystals, which result in drastic changes in the UV spectra of naphthalene, have been found. The study of the IR spectra suggests that there are admixture aniline derivatives of different types, including those with a hydrogen bond between the amino group of an admixture and π-electrons of crystal molecules. Possible arrangements of aniline molecules in naphthalene crystals have been calculated by the method of atom-atomic potentials. The results of the calculation allow one to explain peculiarities of the IR spectra and changes in the UV spectra. The mechanism of structural transformations of admixture centers, which result in cleavage (formation) of the H-bond due to optical excitation (annealing) of the crystal, is suggested.

Key words: admixture center, hydrogen bond, structural transformations, method of atom-atomic potentials, amino group.

The study of structures of admixture centers makes it possible to establish a relationship between properties of real molecular crystals and peculiarities of the interaction between admixture molecules and crystal molecules. Systems in which the external action allows one to change the arrangement of an admixture molecule in the crystal are of special interest. It has been found previously[1] that changes of this type occur in naphthalene crystals with admixtures of aniline and some its derivatives. Light irradiation at low temperatures followed by annealing results in drastic changes in the UV absorption spectra both of admixture molecules and molecules of the crystal located near the admixture. Study of the IR spectra has revealed the admixture centers, in which molecules of the admixture (with the amino group as the proton donor) and naphthalene (with π-electrons as the acceptor) are bonded by H-bonds.

The purpose of this work is to find mechanisms of structural transformations of admixture aniline molecules in the naphthalene crystal. For this purpose, possible structures of admixture centers in the ground state should be primarily determined. The available experimental methods do not allow one to determine reliably the orientation of admixture molecules; however, it can be calculated by the method of atom-atomic potentials.[2] For the systems considered, special attention should be given to considering the possibility of formation of the H bond with π-electrons as the proton acceptor, because these H-bonds are usually neglected in calculations.[2—4]

Results and Discussion

The effect of light irradiation on the UV spectra of admixture crystals of naphthalene is studied. Several derivatives of benzene, thiophene, and pyrrole containing methyl, hydroxyl, and amine groups as well as halogen atoms were used as admixtures. It is found that irradiation followed by annealing exerts a substantial effect on the UV spectra of naphthalene crystals with admixtures containing an amino group.

Figure 1 presents the absorption spectrum in the region of the lowest exciton transition of the naphthalene crystal with the admixture of *p*-bromaniline (C = 1 %) cooled to 4.2 K in dark, A is the lowest exciton band of the crystal (ν_A = 31476 cm^{-1}), I_1 is the admixture band of *p*-bromaniline ($\nu_{max} \cong$ 31200 cm^{-1}). Light irradiation at 100 K for 40 min results in the complete disappearance of the I_1-band and the appearance of a new admixture I_2-band (ν = 31418 cm^{-1}, Fig. 1, *b*). Subsequent short (3 to 5 min) annealing of the crystal at room temperature results in new drastic changes in the spectrum: the I_2-band disappears and a new admixture I_3-band (ν = 30620 cm^{-1}) with the developed phonon wing appears (Fig. 1, *c*). Prolonged (more than 1 day) annealing of the crystal at room temperature results in restoring the initial spectrum (Fig. 1, *a*). Similar changes occur in the spectrum of naphthalene with the admixture of *p*-chloraniline.

For several other admixtures (aniline, *m*-aminophenol, *m*- and *p*-phenylenediamines, *m*-, *p*-, and *o*-toluidines), there are changes in the spectra of local exciton

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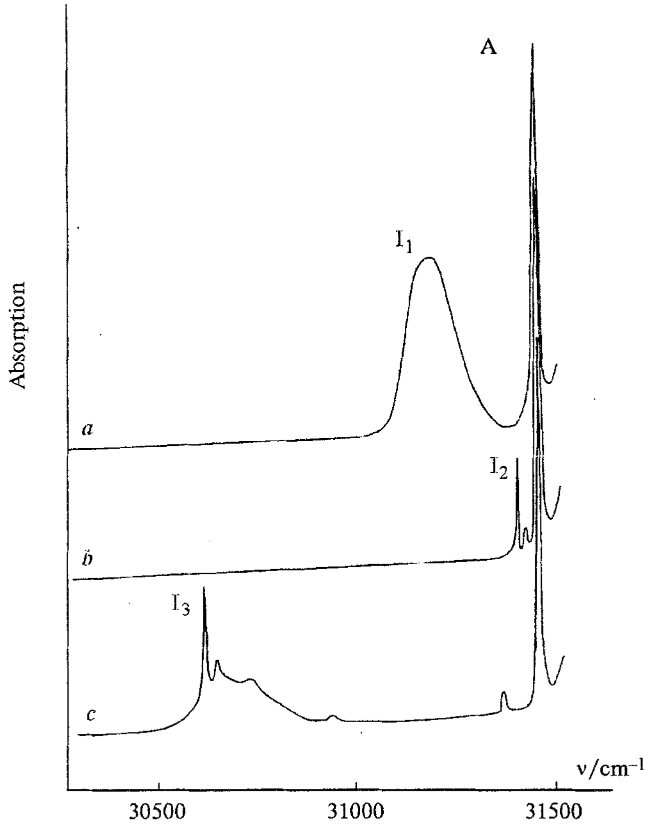

Fig. 1. Absorption spectra of the naphthalene crystal with an admixture of *p*-bromaniline (C = 1 %, T = 4.2 K) before irradiation (*a*); after irradiation (*b*); and after annealing (*c*).

states (X-traps),[5,6] which correspond to the excitation of crystal molecules adjacent to the admixture. These states are sensitive sensors of changes in the interaction within a crystal when an admixture is introduced. Absorption bands of local excitons are usually arranged at the distances of up to 100 cm^{-1} at the long-wave side from the corresponding exciton bands of a pure crystal. It has been shown[5] that the change in the interaction with the charge transfer due to the introduction of an admixture plays a determining role in the formation of local states for the considered transition of naphthalene.

No local bands are observed in the absorption spectrum of naphthalene crystal with the admixture of aniline. Light irradiation results in the appearance of the local L-band at the distance of 11 cm^{-1} at the long-wave side from the exciton A-band (when the temperature of irradiation is 30 K, the growth of the L-band reaches saturation approximately after 15 min). Short annealing at room temperature results in the disappearance of the L-band, and subsequent irradiation exerts no effect on the spectrum. To restore the photosensitivity of the crystal, it should be annealed for long time at room temperature.

The IR absorption spectra of naphthalene crystals with aniline admixtures studied in the range of stretching vibrations of the amino group are presented in Fig. 2 (C = 2 %, T = 300 K). The fact that each admixture exhibits several bands indicates that there are admixture centers of different types. It has been shown[7,8] that the participation of one of the protons of the amino group in the H-bond results in a substantial decrease in the energy of symmetric vibration and a slight decrease in the energy of asymmetric vibration. Involving both protons in the H-bond causes a drastic decrease in the energy of asymmetric vibration and slightly affects the symmetric vibration. Proceeding from this, the IR bands in the spectrum of naphthalene with the admixture of aniline (Fig. 2, *a*) can be interpreted as follows: ν_s = 3404 cm^1 and ν_{as} = 3493 cm^{-1} are related to vibrations of aniline molecules, which are not involved in the H-bond; ν_s = 3386 cm^{-1} corresponds to vibrations of aniline molecules involved in the H-bond through one of the protons of the NH_2 group; ν_{as} = 3468 cm^{-1} and ν_{as} = 3443 cm^{-1} suggest that there are two different admixture centers in which both protons of the amino group are involved in H-bonds.

The concentration studies of the IR spectra (C = 1 to 5 %) show that the bands observed correspond to single admixture centers. Therefore, only π-electrons of naphthalene molecules can act as proton acceptors. The N—H...π-type bonds are weak, which is in good accordance with the shifts in bands observed (Fig. 2). Thus, the results obtained suggest that there are several different types of admixture centers for aniline molecules and its derivatives in naphthalene crystals, and irradiation of crystals followed by annealing makes it possible to perform mutual transformations of these centers.

To elucidate the reasons for phototransformations, possible structures of admixture aniline molecules in naphthalene crystals have been studied by the method of

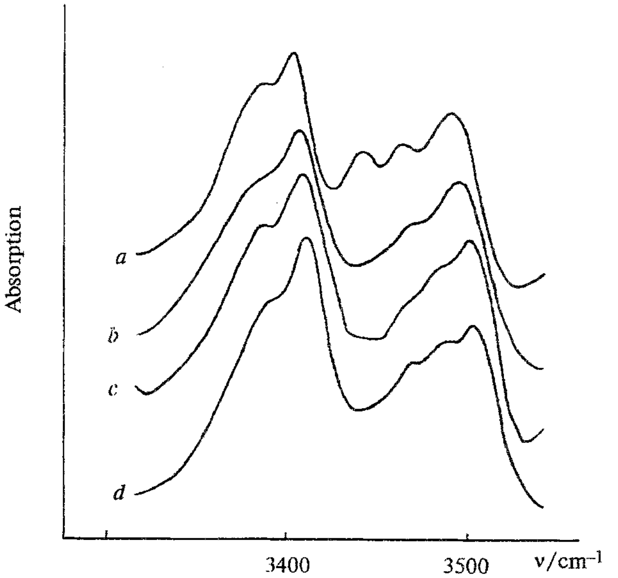

Fig. 2. IR spectra of the naphthalene crystal with admixtures of aniline (*a*); *o*-toluidine (*b*); *p*-chloraniline (*c*); and *p*-bromaniline (*d*). C = 2 %, T = 300 K.

atom-atomic potentials.[2] The structure of a pure naphthalene crystal has been calculated preliminarily with fixed lattice constants (T = 92 K):[9] the energy of the lattice is minimized over three Euler angles, which determine the orientation of molecules in the crystal. The results obtained (φ = 64.4°, φ = 111.9°, θ = 68.7°) agree well with the experimental[10] and previously calculated[11,12] values and depend mainly on the lattice constants used.

To determine the structure of the admixture center, the crystal molecule at position (0,0,0) is replaced by the aniline molecule, and the energy of its interaction with surroundings is minimized relative to its orientation. The positions of adjacent molecules are considered to be fixed. This approximation is appropriate, because it was shown[11] that in the crystal of naphthalene the relaxation of molecules around the vacancy is small (shifts < 0.1 Å and rotations < 2 to 3°). This relaxation around the admixture, which is somewhat smaller in size than the crystal molecule, is still smaller. It was taken into account in the calculations that a free molecule of aniline is nonplanar in the ground state: its energy W has two minima ($\cong -1.5$ kcal/mol) at the values of the angle ω between the planes of the benzene ring and the amino group of ±42° and a maximum (0 kcal/mol) at $\omega = 0°$.[13]

The sum of the energy W and the energy of the interaction between an aniline molecule and surroundings $U = U(\varphi,\theta,\varphi,\Delta a,\Delta b,\Delta c',\omega)$ were minimized over the parameters mentioned (Δa, Δb, and $\Delta c'$ are the shifts of the aniline molecule). The energy U is primarily expressed through a combination of the (exp-6)-type atom-atomic potentials for all interactions, and the possibility of formation of the H-bond involving protons of the amino group is not taken into account. Six different types of admixture aniline molecules **I—VI** in the naphthalene crystal are obtained (Table 1). Possible orientations of the benzene ring of the aniline molecule relative to the arrangement of the molecule-precursor of the crystal are presented in Fig. 3 (two positions of the amino group with $\omega > 0°$ and $\omega < 0°$ are possible for each orientation). It is noteworthy that the changes in the angle ω in the crystal are small (<1°). All six types of admixture centers (Table 1) differ in energy (the difference does not exceed 1 kcal/mol for centers with the same signs).

The possibility of formation of H-bonds with π-systems as proton acceptors is not taken into account, as a rule, in the known calculation schemes.[2—4] For example, it has been determined in the calculation of the structure of the benzene + H_2O complex, using (6-12-1)-type potentials,[4] that protons of a water molecule are arranged at a distance of 3 Å from the plane of the benzene molecule, and an oxygen atom is located at a distance of 3.2 Å. This configuration does not correspond to the known conditions of existence of the H-bond,[14] while the IR spectrum of the complex mentioned[15] indicates that this bond exists.

The following scheme was used in this work for taking into account the possibility of the H-bond formation: the (10—12)-type potential is assumed for the H-bond between a proton of the amino group and π-electrons of the naphthalene molecule. This potential contains the distance R from the proton to the proton-withdrawing center. The choice of the model of the arbitrary withdrawing "center," which presents the

Table 1. Results of the calculation of admixture aniline molecules in the naphthalene crystal ($U_0 = -1.4$ kcal/mol, $R_0 = 2.1$ Å)

Form	U kcal/mol	ω deg	Type of admixture center	Position of the proton-withdrawing molecule	Number of the arbitrary withdrawing "center"	Energy of the H-bond kcal/mol	$R_{H..\pi}$ Å	$R_{N..\pi}$ Å
1	−25.37	−42.1	I				> 3	
2	−25.18	42.3	I				> 3	
3	−25.37	−42.3	II				> 3	
4	−24.92	41.4	II				> 3	
5	−25.37	−42.0	III	(−1/2, 1/2, 0)	1	—	2.82	3.51
6	−25.22	41.6	III	(−1/2, 1/2, 0)	11	—	2.87	3.61
7	−25.59	−41.0	III	(−1/2, 1/2, 0)	1	−0.54	2.54	3.22
8	−25.79	−42.8	IV	(−1/2, 1/2, 0)	1	−1.22	2.22	3.07
9	−24.50	38.4	IV	(−1/2, 1/2, 0)	1	−0.57	2.52	3.00
10	−25.22	39.8	III	(−1/2, 1/2, 0)	11	−0.42	2.63	3.37
11	−25.07	39.4	IV	(−1/2, 1/2, 0) (1/2, 1/2, 1)	2 8	−0.85 −0.40	2.38 2.64	3.05 3.56
12	−23.76	40.8	V	(1/2, −1/2, 0) (1/2, −1/2, 0)	6 4	−1.33 −0.89	2.17 2.36	2.90 2.88
13	−24.42	−42.1	VI	(1/2, −1/2, 0)	4	−0.86	2.37	3.10
14	−24.02	42.5	VI	(1/2, −1/2, 0)	4	−1.24	2.21	3.04

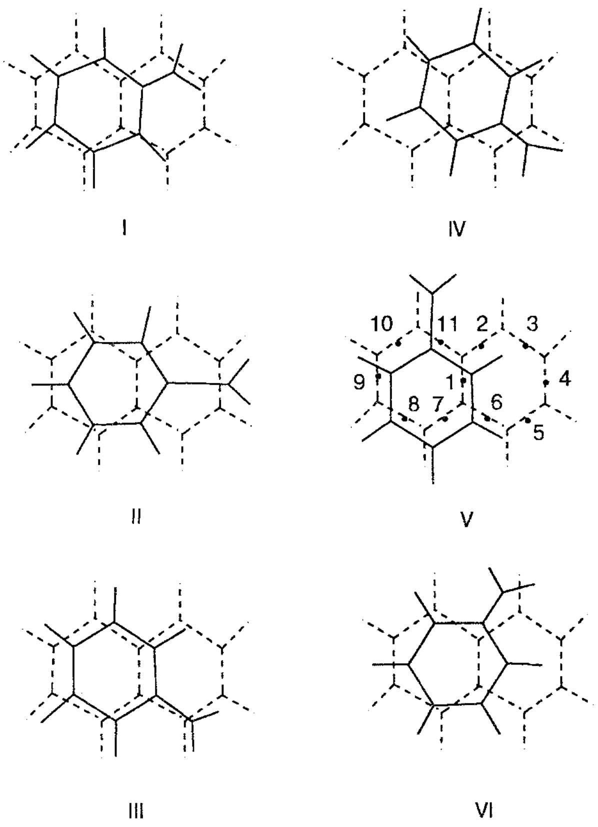

Fig. 3. Schematic presentation of possible orientations of the aniline molecule relative to the arrangement of its molecule-precursor in the naphthalene crystal.

π-system, is significant. In the known complexes with the H-bond with benzene, protons are oriented either to the center of the benzene ring or to the center of one of C—C-bonds.[4,16–18] In addition, π-systems are characterized by a smooth change in the Coulomb potential along the aromatic ring.[18] These facts allow one to suggest several method for choosing R as the distance from a proton to (1) the center of the naphthalene molecule; (2) to the center of one of its benzene rings; (3) to its plane; (4) to the center of one of C—C-bonds of the molecule (the numbering of the arbitrary proton-withdrawing "centers" is presented in Fig. 3, V).

The potential for the H-bond substitutes the sum of the (exp-6)-type potentials for the interaction between a proton of the amino group and all carbon atoms of the corresponding naphthalene molecule. This substitution was performed in the cases when, first, it provided a decrease in the energy of the system and, second, the distance R satisfied the condition of the existence of the H-bond. It should be taken into account that R is the distance from a proton to the arbitrarily chosen withdrawing center, but not to the carbon atom. Taking into account the known conditions of the existence of the H-bond,[14] the distance R_0 = 2.7 Å is accepted as a critical distance. This condition is rather rigorous, because in the known H-complexes with benzene molecule[16,17] the minimum distance between a proton and carbon atoms is 2.6 to 2.8 Å. It should be noted that for the system considered in the majority of cases, this criterion is not a determining one in calculations of structures of admixture centers; however, it becomes extremely important for estimating energy barriers between various admixture centers.

The (10—12)-type potential of the H-bond is characterized by the minimum energy U_0 corresponding to the distance R_0. The choice of these parameters is based on the following facts: (1) the enthalpy of formation of the H-bond between aniline and benzene is −1.64 kcal/mol[19] or −1.19 kcal/mol[20] according to different data (naphthalene is similar to benzene in proton-withdrawing properties[21]); (2) the R_0 distance is close to 2.0 to 2.2 Å in the known potentials of the N—H...X-type H-bond;[3,4] and (3) the energy of the interaction between a proton and all carbon atoms of the naphthalene molecule (using parameters from Ref. 22) reaches −0.4 kcal/mol. Starting from this, the potentials of the H-bond with U_0 = −1.0 to −1.8 kcal/mol and R_0 = 2.0—2.2 Å are used in the calculations.

For the system considered, the energy of the H-bond is a small addition to the energy of the dispersion interaction between the admixture and surroundings. Therefore, the H-bond is realized when conditions of its formation do not contradict the packing of molecules in the crystal, which is determined by the dispersion interaction (in the case of the strong H-bond, the existence of the solid solution of substitution becomes conjectural). It is reasonable that in the case of admixtures, which are smaller than crystal molecules, there are more possibilities for the appearance of the H-bond. Taking into account the possibility of formation of the H-bond between protons of the amino group and π-electrons of crystal molecules allows us to find several new admixture centers. It should be mentioned that in all cases the plane of the benzene ring of the admixture is close to the plane in which the molecule-precursor was located, and the ω angle changes insignificantly.

When proton-withdrawing properties are ascribed to the center of naphthalene molecules, the H-bond is formed only with crystal molecules at the position (−1/2, 1/2, 0), which is inherent in three admixture centers 7—9 (Table 1). It is noteworthy that centers 7 and 8 are energetically more favorable than forms 1—6 without H-bonds.

The use of other methods for choosing R makes it possible to take into account the extended character of the proton-withdrawing π-system. When R is determined as a distance from a proton to the plane of the corresponding molecule of naphthalene, the results of calculations for admixture centers 7—9 are similar to those presented in Table 1. In addition, admixture centers, in which aniline molecules are H-bonded to crystal molecules at the position (1/2, −1/2, 0), can also be predicted. However, the use of this method is

Table 2. Energies of admixture centers at different parameters of the H-bond potential

$\frac{U_0}{\text{kcal/mol}}$	$\frac{R_0}{\text{Å}}$	Center						
		7	8	10	11	12	13	14
−1.4	2.1	−25.59	−25.79	−25.22	−25.07	−23.76	−24.42	−24.02
−1.8	2.1	−25.79	−26.15	−25.35	−25.44	−24.41	−24.69	−24.39
−1.0	2.1	−25.44	−25.46	−25.11	−24.72	−23.13	−24.20	—
−1.4	2.0	−25.42	−25.53	—	−24.71	−23.28	−24.20	−23.76
−1.4	2.2	−25.82	−26.00	−25.41	−25.50	−24.13	−24.68	−24.26

inconvenient, because it requires introducing artificial restrictions on the shift of a proton along the plane of the molecule of naphthalene.

When R is chosen as the distance from a proton to the center of one of the benzene rings of the naphthalene molecule, admixture forms 7 and 8 remain the most stable, and their analogs with a H-bond with the molecule (1/2, −1/2, 0) also appear. The disadvantage of this method is the uncertainty that occurs somewhat in the cases when a proton is located above the center of the naphthalene molecule. Due to this arrangement, form 7, in which a proton is approximately above the center of one of the benzene rings, becomes more favorable than structure 8, in which a proton is located approximately in the middle of the distance between centers of benzene rings.

These disadvantages of two methods presented can be to a great extent eliminated when R is determined as a distance to one of centers of C—C-bonds of the naphthalene molecule. For a proton of the amino group involved in the H-bond, the withdrawing "center" providing the minimum energy in the corresponding naphthalene molecule was found by sorting out. It turned out that forms 7 and 8 (Table 1) are unchanged for such a method. Admixture center 9 is transformed to analog 11 in which both protons participate in H-bonds with different crystal molecules. Additional admixture centers 10, 12—14 with H-bonds at the positions (−1/2, 1/2, 0) and (1/2, −1/2, 0) appear (Table 1).

Thus, this method of calculation allows one to find seven admixture centers with H-bonds. The corresponding orientations of the benzene ring of the admixture are schematically presented in Fig. 3 (III—VI). It is significant that admixture forms 7 and 8 are the most stable for all four methods of determining R.

The accepted scheme of taking into account H-bonds does not allow one to calculate values of energy barriers between different admixture centers. However, some estimations are possible. Let us note first that all admixture centers presented in Table 1 (except 9 and 11) are separated by energy barriers.

Since parameters of the H-bond potential used in this work are estimating, it is necessary to analyze the effect of changes in these parameters on the results of calculations. It is noteworthy that varying the H-bond potential exerts a slight effect on the arrangement of the admixture in the crystal, and the stronger the H-bond the smaller the effect.

The energies of admixture centers at various values of U_0 and R_0 are presented in Table 2. It is reasonable that the energies of admixture forms with longer H-bonds are more sensitive to changes in potential. The disappearance of center 10 at $U_0 = -1.4$ kcal/mol and $R_0 = 2.0$ Å is caused by the fact that R is greater than 2.7 Å. When $U_0 = 1.0$ kcal/mol and $R_0 = 2.1$ Å, the energy barrier between forms 14 and 2 disappears, which results in the disappearance of center 14. It is important that the main admixture structures are retained and centers 7 and 8 remain the most stable at all parameters of the H-bond presented in Table 2.

Let us compare the results of calculations to the experimental data. The IR bands observed (Fig. 2) can be interpreted in the following way: $\nu_s = 3404$ cm^{-1} and $\nu_{as} = 3493$ cm^{-1} are related to admixture centers 1—6 without H-bonds; $\nu_s = 3386$ cm^{-1} corresponds to centers 8 and 14 ($H \cong -1.2$ kcal/mol); and $\nu_{as} = 3468$ cm^{-1} and $\nu_{as} = 3443$ cm^{-1} are related to centers 11 and 12 in which both protons of the amino groups are involved in H-bonds; the bands that belong to centers 7 and 10 are probably superimposed on the bands at $\nu_s = 3404$ cm^{-1} and $\nu_s = 3386$ cm^{-1}, respectively. The estimations of content of different admixture centers, assuming that the energy distribution is exponential, show that the intensities of the IR bands observed at room temperature agree qualitatively with the interpretation suggested.

Now let us consider the transformations of the UV spectra. Cooling to 4.2 K results in the fact that nearly all admixture molecules are transformed to the most energetically favorable form 8. In this case, the absence of the local band in the spectrum can be explained by the existence of the H-bond. For example, in H-complexes the lowest singlet transition is several tens cm^{-1} shift toward the short-wave range.[4] In addition, for the transition considered, the position of the local band is determined by the effect of states with a charge transfer between molecules of the crystal and the admixture,[5] and the H-bond can change substantially these states.[23] Finally, the H-bond can dramatically enhance the electron-phonon interaction, which results in blurring of the local band.

The molecule of aniline in the excited or ionized state is planar[24] ($\omega = 0°$). This noticeably degrades the conditions of existence of the H-bond in the naphthalene crystal and results in its breaking. It can be assumed that the aniline molecule in the excited state is transformed from form 8 to variety 5, which has no hydrogen bond. The local band, whose energy agrees well with that predicted by the theory of local states for several benzene derivatives in the naphthalene crystal,[5] appears in the spectrum.

Short annealing of the crystal transforms the admixture from form 5 to the energetically more favorable variety 7. These centers are characterized by similar orientations of admixture molecules (Fig. 3, III) and are separated with a small energy barrier. At the same time, molecular orientations in admixture centers 7 and 8 differ substantially (Fig. 3, III and IV). Therefore, prolonged annealing of the crystal is necessary to return the admixture to the initial state 8.

Thus, taking into account the possibility of formation of the H-bond between the amino group of the admixture and π-electrons of crystal molecules allows one to explain both the changes in the UV spectra observed and specific features of the IR spectra of the naphthalene crystal with the admixture of aniline. The results obtained suggest that the schemes of atom-atomic potentials should be supplemented by potentials describing H-bonds with π-systems as proton acceptors.

Experimental

Organic substances were purified by zone melting or multiple sublimation. The weighted concentration of an admixture was 1 to 5 %. Admixture crystals of naphthalene were grown by sublimation (the width d = 1 to 10 μm) or from melt (d = 300 to 500 μm). UV spectra were recorded on a DFS-13/2 spectrograph, and IR spectra were measured on an IKS-29 spectrograph. Crystals were irradiated by nonfiltered light from a DKSSh-120 lamp at 4.2 to 100 K and a maximum exposure of 1 h.

Previously published parameters of atom-atomic potentials[22,25] and structures of naphthalene[26] and aniline[27] molecules were used in calculations of structures of admixture centers. Interactions at the distances shorter than 12 Å were taken into account. Positions of admixtures were calculated with the accuracy of 0.01 Å and orientations were calculated with the accuracy of 0.1°.

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