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THE THEORY OF THE ABSORPTION SPECTRA OF MOLECULAR CRYSTALS

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I. THE PROBLEM

In the examination of the optical characteristics of molecular crystals, it appears to us that the combination of individual molecules is arranged in a lattice characteristic for the given crystal.

In the first approach we will consider that the molecules are firmly secured in the equilibrium condition and have a fixed space orientation (if the molecules are asymmetrical). The heat motion of the molecules (and of the atoms within the molecules) leading to the appearance of vibrational-rotational structures can be computed indirectly, as is done in the examination of molecular spectra.

As is known, there can always be distinguished within a molecule groups of electrons the energy states of which determine the absorption of the molecules in the long-wave region of the spectrum and whose wave functions are weakly overlapping with the wave functions of the remaining electrons. We will call those electrons "optical." In many organic compounds such electrons take the form of the so-called π electrons.

We shall assume that the crystal is made of the same kind of molecules, each of which has S "optical" electrons. The state of k molecules will be determined by the wave function which is dependent on the coordinates and spins of these electrons. Such a function can be presented as the product of the functions ω_k and χ_k which are dependant only on the coordinates and spins of those electrons, respectively.

$$\Psi_k = \omega_k \chi_k$$

Let H_k be the energy operator of k molecules, and V_{kn} be the operator of the energy of the reaction of k and n molecules. Then the wave functions and the

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energy levels (E) of the stationary condition of the whole crystal will be determined by Schroedinger's equation

$$\left(\sum_{k} H_k + \sum_{k<l} V_{kl} - E\right)\Phi = 0 \qquad (1)$$

Here the summation is extended through all n molecules making up the crystal. The wave function depends on the coordinates of all the electrons (we shall deal only with "optical" electrons; hereafter, we shall omit the word "optical"); coordinates of the molecules and their space orientations will enter into it as parameters. Later we will designate the position and orientation of the molecules in the lattice by one symbolic vector, R.

To solve the problem of the absorption and radiation of light by crystals in the visible and ultraviolet regions of the spectrum, we will be interested in the normal and primary excited state of the crystal.

Let Φ_0 be the wave function of the crystal when all the molecules are found in the normal state. The wave function Φ_0 can be presented in a neutral approach as an anti-symmetrical product of wave functions φ_i of the normal state of the individual molecules

where

$$\Phi_0 = \frac{1}{\sqrt{(SN)!}} \sum_{\nu} (-1)^{\nu} P_{\nu}\, \psi, \qquad (2)$$

$$\psi = \varphi_1 \varphi_2 \cdots \varphi_N ; \qquad (3)$$

P_{ν} = one of the possible (S N)/ rearrangements of the electrons. The summation $\sum_{\nu}$ occurs in all possible rearrangements of the electrons. All φ_i functions are assumed to be normalized and real. In spite of this we discard the integrals of the non-orthogonal (overlapping) wave functions of the adjacent molecules.

The energy of the crystal in the first approximation is determined from (1) after the substitution of (2), multiplying by (3) and integrating along all the coordinates of the electrons:

$$E^0 = \sum_{k} E_k^0 + \sum_{k<l} \Big\{ \int \varphi_k^2(I) V_{kl} \varphi_l^2(II)\, d\tau -$$

$$- \sum_{\mu} \int \varphi_k(I) \varphi_l(II) V_{kl} \varphi_{kl}(II) \varphi_k(I)\, d\tau \Big\}, \qquad (4)$$

Here φ_k (I) and φ_l (II) appear as wave functions of the molecules k and l at a certain distribution of the electrons in the molecules; φ_k (II) and φ_l (I) = functions in the rearrangement between molecules k and l of any pair of electrons; and the sum $\sum_{\mu}$ covers over all possible rearrangements of electron pairs between the k and l molecules.

Now let

$$\psi_n = \varphi_1 \varphi_2 \cdots \varphi_n' \cdots \varphi_N \qquad (5)$$

be the wave function of the electrons when n molecules are found in undegenerate excited state and all molecules are sufficiently removed from one another. When the molecules converge (to construct the crystal), the excitation in n molecule will no longer be localized, but will be transferred from one molecule to another [1,2]. Because of this, the wave function of the excited state of the crystal, which is antisymmetrical relative to the rearrangement of the electrons, can be presented in the superposition state:

$$\Phi_n = \frac{1}{\sqrt{(SN)!}} \sum_{\nu} (-1)^{\nu} P_{\nu} \psi_n \qquad (6)$$

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with a certain amplitude a_n, [illegible] the coordinates R of all the molecules.

$$\Phi = \frac{1}{\sqrt{N}} \sum_n a_n(R)\, \phi_n, \tag{7}$$

where $|a_n(R)|^2$ determines the probability that, at a given distribution of the molecules, n molecules will appear in an excited state.

Substituting (7) in (1), multiplying by ψ_m and integrating along all the coordinates of the electrons we get a system of algebraic equations for the determination of a_n and the energy E of the crystal.

$$\sum_n{}' a_n M_{mn} - \varepsilon a_m = 0, \quad m = 1, 2, \ldots N. \tag{8}$$

The summation is extended through all molecules with the exception of m; the matrix element

$$M_{nm} = \int \varphi_m'(I)\, \varphi_n(II)\, V_{mn}\, \varphi_m(I)\, \varphi_n'(II)\, d\tau - \\ - \sum_{\mu} \int \varphi_m'(I)\, \varphi_n(II)\, V_{mn}\, \varphi_m(II)\, \varphi_n'(I)\, d\tau \tag{9}$$

characterizes the change of excitation between n and m molecules:

$$-\varepsilon = E_m' + \sum_k{}' \Big\{ E_k^0 + \int \varphi_m'^2(I)\, V_{ml}\, \varphi_k^2(II)\, d\tau - \sum_{\mu} \int \varphi_m'(I)\, \varphi_k(II)\, V_{ml}\, \varphi_m'(II)\, \varphi_k(I) \\ \times d\tau \Big\} + \sum_{k<l}{}' \Big\{ \int \varphi_k^2(I)\, V_{kl}\, \varphi_l^2(II)\, d\tau - \sum_{\mu} \int \varphi_k(I)\, \varphi_l(II)\, V_{kl}\, \varphi_k(II)\, \varphi_l(I)\, d\tau \Big\} - E, \tag{10}$$

The prime superscript in the sum shows that the summation is extended through all the molecules except m.

Subtracting from E, which was determined from (10), the energy of the normal state E_0 (4), we get the energy of the excited crystal

$$\Delta E = \Delta E_m + D + \varepsilon, \tag{11}$$

where $\Delta E_m = E_m' - E_m^0$ is the excitation energy of one of the molecules

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and

$$D=\sum_{k}\Big\{\int \varphi_m^1(I)V_{mk}\varphi_k^2(II)\,d\tau-\int \varphi_m^2(I)V_{km}\varphi_k^3(II)\,d\tau-$$

$$-\sum_{k}\Big[\int \varphi_m'(I)\varphi_k(II)V_{mk}\varphi_m'(II)\varphi_k(I)\,d\tau-$$

$$-\int \varphi_m(I)\varphi_k(II)V_{mk}\varphi_m(II)\varphi_k(I)\,d\tau\Big]\Big\}. \quad (12)$$

Thus the excitation energy of a crystal is distinguished from the excitation energy of a molecule by two terms, D and ε .

To calculate ε it is necessary to solve the system of homogenous equations (8) involving a_n . With an ideal periodical distribution of molecules, the coefficients a_n can be distinguished from one another only by the phase since it is just as probable to find any molecule in an excited state. Accordingly, we will look for the solution of the system of equations (8) by taking

$$a_n = e^{ikn}, \quad (13)$$

where we will assume n to be the radius vector characterizing the condition at the center of n molecules in the crystals and k the wave vector characterizing the excitation wave in the crystal.

Substituting (13) in (8) and selecting for the basis the coordinates in the m molecule, we get

$$\varepsilon=\sum_{\ell=1}^{N-1} e^{ik\ell}M_{0\ell}, \quad (14)$$

where $\ell=n-m$. As is clear from (14), for each descrete natural energy value of the electron in the isolated molecule, there is a corresponding whole band of thickly distributed natural values of the electron energies in the crystal. The width of this band is determined by the values of the integrals $M_{0\ell}$ characterizing the transfer of excitation energy from 0 to ℓ molecules. For molecular crystals, these integrals, even for adjacent molecules, are small (in the order of 0.01 eV or smaller).

For the calculation of matrix elements (9) we make use of a series separation, in steps of $1/r_{nm}$, of the classical energy of reaction V_{nm} between two molecules. If we are limited only by the first term of the series separation (i.e., dipole-dipolar reaction) then

$$V_{nm}=-\frac{e^2}{r_{nm}^3}\sum_{i,j}\{2z_{in}z_{jm}-x_{in}x_{jm}-y_{in}y_{jm}\}, \quad (15)$$

where x_{in}, y_{in}, z_{in} , and x_{jm}, y_{jm}, z_{jm} are the coordinates of the electrons i and j in the two molecules, corresponding to the system of coordinates which are separated in the center of the molecules, so that the line joining the centers of the molecules coincides with the Z axes of both systems.

By subtituting (15) in (9), we will immediately see that, for dipolar transfers in molecules, the first integral only will have a practical value which determines the resonance reaction between the two molecules. With this approximation we will get the matrix element (9) in the following form

$$M_{nm}=-\frac{e^2}{r_{nm}^3}\left|\int \varphi' r\varphi\,d\tau\right|^2\{2\cos\theta_m^z\cos\theta_n^z-$$

$$-\cos\theta_m^x\cos\theta_n^z-\cos\theta_m^y\cos\theta_n^y\}, \quad (16)$$

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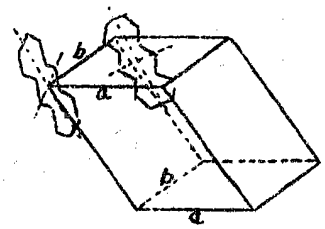
where $e\int \varphi' r \varphi d\tau$ is the matrix element of the vector of the electrical moment, determining the quantum transfer within the molecules; $\cos\theta^x_m, \cos\theta^x_n \ldots$ are the cosines of the angles formed by the vectors of the electrical moments in the molecules m and n, corresponding to the axes of the coordinates.

For prohibited dipolar transfers $\int \varphi' r \varphi d\tau = 0$. In this case it is necessary to calculate in (9) the reaction of a much higher order (quadrupole, etc.). Then it is not necessary to discard the second term in (9), since in certain cases it will have a value similar in magnitude to the first term.

II. ENERGY TERMS OF MOLECULAR CRYSTALS OF A MONOCLINIC SYSTEM

We will use the results obtained in the foregoing section for molecular crystals of the anthracene, naphthalene and other types which crystallize into a monoclinic prismatic system with a cubic group symmetry C_{2h}. A single nucleus of such a crystal contains two molecules, the arrangement and orientation of which are well known.



Space Distribution of the Molecules of Anthracene

The above figure is a diagram of the space distribution of the molecules of anthracene according to Robertson [3]. The molecules of anthracene are flat and have a rhombic symmetry. In the crystal the molecules are arranged in cleavage planes (plane ab) so that the centers of the molecules occupy the centers and corners of the faces ab. The molecules found in the center of the plane have a space orientation different from the orientation on the molecules found in the corners of the plane.

We will consider only the reaction between the molecules which lie within the cleavage planes of the crystal (plane ab), since the forces of reaction between molecules of different cleavage planes is small in comparison with the forces acting between the molecules found in one cleavage plane.

We will introduce the basic vectors a and b of the cleavage plane of the crystal lattice. Then the state of any molecule in the cleavage plane will be characterized by the vector

$$l = \frac{a}{2} n + \frac{b}{2} m \tag{17}$$

where n and m simultaneously take either even or odd, positive or negative integer values. Molecules whose state will be characterized by even numerical values of n and m will be called "even" molecules. The orientation of all even molecules in space is the same (transferable-equivalent molecules). Molecules whose state is characterized by odd values of n and m will be called "odd." All odd molecules are transferable-equivalent among each other and have an orientation different from even molecules.

If we are going to calculate the change in excitation only between adjacent molecules, then the correction of (14) to molecular terms can be written in the following way

$$\varepsilon = 2A\cos 2\eta + 2B\cos 2\xi + 4C\cos\eta\cos\xi \tag{18}$$

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where $\eta = k_y b/2$, $\xi = k_x a/2$; A = matrix element (16) of reaction between the two closest molecules along the axis b (either odd or even); B = matrix element (16) of reaction between the two closest molecules along the axis a (either even or odd); C = matrix element (16) of the reaction between the two closest transferable-nonequivalent molecules (odd and even).

The wave function, corresponding to the energy (18), will appear as

$$\Phi_{\xi\eta} = \frac{1}{\sqrt{N}} \sum_{n,m} e^{i(\xi n + \eta m)} \phi_{n,m}, \tag{19}$$

where the summation is extended through all the even and odd values of n and m characterizing the condition of the molecules:

$$\phi_{nm} = \frac{1}{\sqrt{(3N)!}} \sum_{\nu} (-1)^{\nu} P_{\nu} \psi_{nm},$$

$$\psi_{nm} = \varphi_{11} \varphi_{22} \varphi_{13} \cdots \varphi'_{nm} \cdots$$

To determine the rules of selection and the polarizations of additional transitions in the crystal from a normal condition Φ_0 to an excited state $\Phi_{\xi\eta}$, it is necessary to calculate the matrix element

$$R_{\xi\eta} = \int \Phi_{\xi\eta}\, r\, \Phi_0\, d\tau, \quad r = \sum_{n,m} r_{n,m}. \tag{20}$$

Substituting the functions (19) and (2) in (20) we will see that the matrix element (20) will be equal to zero for all values of ξ and η, except

$$\left.\begin{aligned} &(\alpha)\ \xi = \eta = 0, \\ &(\beta)\ \xi = 0,\ \eta = \pi\ (\text{or } \xi = \pi,\ \eta = 0). \end{aligned}\right\} \tag{21}$$

Thus the optical transitions (of the dipole type) in our crystal are basically in the excited state, characterized only by two pairs of values of ξ and η. Namely, transitions are possible in the following states

$$\Phi_\alpha = \frac{1}{\sqrt{N}} \left\{ \sum_{\substack{nm \\ \text{even}}} \phi_{nm} + \sum_{\substack{nm \\ \text{odd}}} \phi_{nm} \right\}, \tag{22}$$

$$\Phi_\beta = \frac{1}{\sqrt{N}} \left\{ \sum_{\substack{nm \\ \text{even}}} \phi_{nm} - \sum_{\substack{nm \\ \text{odd}}} \phi_{nm} \right\}. \tag{23}$$

Corresponding to this we obtain two types of matrix elements, R_α and R_β. Changes with the matrix element R_α, except zero, will correspond to the change of energy (11) in the crystal

$$\Delta E_\alpha = \Delta E_m + D + 2A + 2B + 4C. \tag{24}$$

The change with the matrix element R_β, except zero, will correspond to the change of the energy of the crystal

$$\Delta E_\beta = \Delta E_m + D + 2A + 2B - 4C. \tag{25}$$

As was shown in our previous work [4], in naphthalene molecules (as well as anthracene) belonging to the group symmetry D_{2h}, the excited state of π electrons can belong to four unexcited representations A_{1g}, A_{2g}, B_{1u}, and B_{2u} of group symmetry B_{2H}.

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The normal state of these molecules [illegible] to the unexcited fully-symmetrical representation A_{1g}. Optical changes with normal conditions are permissible only in the excited states B_{1u} and B_{2u} (with corresponding polarizations along the long and short axes of the molecules). Changes in states A_{1g} and A_{2g} are prohibited.

Knowing the symmetry of the wave functions and the rules of selection and polarization of electron transfers in the molecule, by using the group theory to determine the symmetrical characteristics of the corresponding wave functions of the crystal, there can be determined the rule of selection and polarization of the spectrum lines of the crystal.

It is natural that the character of the excited states of the crystal will be dependent on the corresponding type of excited molecular state. Because of this, the wave functions of the excited state of the crystal will be represented by the symbols $\Phi(\Gamma_i)$, where Γ_i will indicate the nature of the unexcited representation of the excited state of the molecule.

The characters of the unexcited representation of a group symmetry C_{2h} of a crystal, together with the representation of conversion characteristics of the components of the radius-vector (r_a, r_b, r_c), are given in the following table.

	E	C_2^b	i	σ^b	
A_g	1	1	1	1	
A_u	1	1	- 1	- 1	r_b
B_g	1	- 1	1	- 1	
B_u	1	- 1	- 1	1	r_a, r_c

We will notice that both operation (E) and inversion (i) coincide in the molecule and crystal. The operation of symmetry in the crystal C_2^b and σ^b corresponds to the rearrangement of even molecules with the odd, the ensuing rotation of the molecule around its short axis being 180 degrees (i.e., operation C_2^y of the molecule). Consequently, the reflection in the plane is perpendicular to this axis (operation σ^y of the molecule). Thus using the table of characters of the unexcited group representation of the symmetry of molecules, we obtain the following conversion characteristics of the wave function $\Phi_\alpha(B_{1u})$ of the crystal;

$$E\Phi_\alpha(B_{1u}) = \Phi_\alpha(B_{1u});\ C_2^b\Phi_\alpha(B_{1u}) = -\Phi_\alpha(B_{1u});$$

$$i\,\Phi_\alpha(B_{1u}) = -\Phi_\alpha(B_{1u});\ \sigma^b\Phi_\alpha(B_{1u}) = \Phi_\alpha(B_{1u}).$$

Comparing the obtained results with the characters in the above table, we will see that the wave function of the crystal is converted similarly to the unexcited representation $\Phi_\alpha(B_{1u})$ of group symmetry C_{2h}, which we will write shortened thus:

$$\Phi_\alpha(B_{1u}) \sim B_u.$$

Similarly we can determine the conversion characteristics of the remaining functions:

$$\Phi_0(A_{1g}),\ \Phi_\alpha(A_{1g}),\ \Phi_\beta(A_{2g}) \sim A_g,$$

$$\Phi_\alpha(A_{2g}),\ \Phi_\beta(A_{1g}) \sim B_g,$$

$$\Phi_\alpha(B_{2u}),\ \Phi_\beta(B_{1u}) \sim A_u,$$

$$\Phi_\alpha(B_{1u}),\ \Phi_\beta(B_{2u}) \sim B_u.$$

Using the group theory, we can now show the rules of selection and polarization of the corresponding optical dipolar changes. All changes from the normal

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state to an agitated state of crystals with wave functions $\Phi_a(A_{1g})$, $\Phi_a(A_{1g})$, and $\Phi_b(A_{2g})$ are forbidden. Changes to all remaining planes are permitted. Thus the transfers in the crystal are not permitted if they correspond to the prohibited changes in the molecule, and permitted if they correspond to the permissible changes in the molecule.

For each permissible transfer in the molecule there are two corresponding permissible changes in the crystal. In other words, the energy term of the molecule in the crystal is divided into two terms which are distinguished from each other by the polarization. One of the terms is polarized so that the vibration of the electrical vector is aligned with the axis b in the crystal; that of the other, with the plane perpendicular to axis b. The division of the molecular terms is conditioned by a dissimilar space orientation of anisometric molecules in the crystal. If the molecules had a similar orientation, then the division (of the type investigated here) would be absent; there would only be a shifting of molecular terms.

The amount of the division of a molecular term is

$$\Delta = BC, \tag{26}$$

The division of the terms corresponding to the prohibited changes in the molecule, is always less than the division of the permissible terms.

Our results are found to be in contradiction with those of V. L. Herman [5] in that the possibility of division of the energy levels in the naphthalene crystal is excluded for separate molecules.

Both crystal terms are shifted relative to the corresponding molecular term by the amount

$$\delta = D + 2A + 2B \tag{27}$$

As the dimension is displaced, so is the dimension of division dependent on the type of electrical transfer in the molecule.

In the given work we examine the change of undegenerate excited molecular states in a molecular crystal. If in the molecule there is a degenerate excited plane, then it may be removed by the insertion in the crystal of another degenerate symmetry. This will lead to a division of the molecular terms similar to the division of atomic terms which has already been investigated qualitatively by Bethe [6]. Each of the divided (in consequence of being removed) degenerate components can still be divided in the crystal due to the effect which was examined in the given work.

A characteristic peculiarity of molecular crystals is that the spectrum of the crystal (at absorption as well as fluorescence) at very low temperatures consists of sharp, often very narrow, bands. This was shown in connection with the work of investigating the spectra of crystals at the temperature of liquid hydrogen by L. V. Chroimov and A. F. Erikhrt'ko [7].

These spectra, it appeared, were found to be in contradiction with the usual appearance of the zone arrangement of the energy levels of the crystals. Although the forces of reaction in molecular crystals are small, the width of the energy zone in such a crystal, in size, should differ only a little from that of the energy of sublimation, i.e., should be within hundredths of the reciprocal of centimeters. The absorption spectrum of the naphthalene crystal consists of a group of narrow bands [8], some of which appear as radiations due to the width of the line.

As was shown in this work, the discrete nature of the absorption line is explained not by the narrowness of the energy levels of the crystal but by the rules of selection of the optical transfers in the crystal. It is possible that the optical transfers occur only at fully determined values of the wave terms.

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In crystals, such as anthracene, [illegible] changes can occur only between a basic level and the upper or lower edge of the energy zones in the excited state of the crystal. A quantitative calculation of the absorption spectra of monocrystals of anthracene and naphthalene and a comparison with experiments will be done in a following project.

In conclusion, I express my thanks to Professors S. I. Pekar and A. F. Prikhot'ko for their helpful discussion and interest in the work.

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