

Band electron spectrum and optical properties of KDP-crystals under the external hydrostatic pressure

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The electron spectrum of the KDP-type crystals has been investigated as a function of the external hydrostatic pressure using the tight-binding approximation. The joint density of electron states, real and imaginary parts of the dielectric permeability, refraction indices, the gyration coefficient, absorption and reflection coefficients for different polarizations of light are determined. Their pressure and frequency dependencies are investigated. The results are discussed by comparing them with the experimental data on piezooptic coefficients. The anomalous behaviour of the optical constants at the pressure $p \simeq 17$ kbar is due to the transformation of the hydrogen bond potential from a double minimum one to a single minimum one, where the proton is localised at the midpoint of the hydrogen bond.

Key words: *electron spectrum, hydrostatic pressure, optical properties*

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1. Introduction

The physical properties of ferroelectric systems with hydrogen bonds are mainly functions of the bond length and the character of proton motions. Above T_c , the protons move in a symmetric double well potential along the $O - H - O$ bonds. Below the ferroelectric transition temperature T_c , an ordering of protons in one of these two minima takes place. The most important effect, connected with the decreasing of the bond length, is the decreasing and ultimate vanishing of the transition temperature T_c [1]. So, it is interesting to investigate the physical properties of such systems with a change of the structural parameters of hydrogen bonds, which gives us a possibility to examine the mechanism of the ferroelectric phase transition. One can change the structure of hydrogen bonds by external pressure, deuteration or other isomorphous changes, for example, substitution of

KH₂PO₄ by RbH₂PO₄, KH₂AsO₄, etc. Application of pressure is the simplest of them, because the system itself does not change. It is known (see [2,3]) that both KDP and DKDP show a large negative pressure dependence of T_c , and T_c of KDP falls to 0K at 17 kbar. According to Nelmes and co-authors [4–9], above 17 kbar, at 0K, the along-bond (zero-point) thermal motion of the H atom about each site (i. e. the two minima of the potential well with the distance δ between them), $U^{22}(\text{H})$ is larger than $(\delta/2)^2$. Strictly, $U^{22}(\text{H})$ is a mean-square amplitude along the y -axis; but this axis is very close to the line joining the two H sites. There then seems to be a simple structural explanation for the loss of the ordered phase that does not necessarily entail tunnelling effects: above 17 kbar, the thermal amplitude of the H atom is always greater than $\delta/2$, the distance from each of the sites to their midpoint, and it seems reasonable to expect that the H atom cannot be localised on one site only. The experimental data of [4–9] describe the changes of the KDP structure with pressure in the pressure region $1 \text{ bar} \leq p \leq 17 \text{ kbar}$. In paper [12], similar investigations for the pressures $1 \text{ bar} \leq p \leq 54 \text{ kbar}$ were carried out, but the proton positions were not determined. Thus, the behaviour of the protons in the KDP structure at pressure $p > 17 \text{ kbar}$ is not experimentally studied. According to [10,11], at further decrease of the bond length (for example, with the increase of pressure, for $p > 17 \text{ kbar}$), the δ value falls to zero. This change may be either abrupt [11] or smooth but in the latter case δ rapidly nonlinearly falls to zero [10]. According to [10,12], this change is expected in the pressure region $17 \text{ kbar} \leq p \leq 27 \text{ kbar}$. The value of pressure at which $\delta \rightarrow 0$ can be determined only experimentally. It is interesting to calculate the changes of optical functions which are induced by an abrupt change of $\delta \rightarrow 0$. We have taken $\delta \rightarrow 0$ at $p = 17 \text{ kbar}$ in our calculations of optical constants. The results will not change qualitatively if we put $\delta \rightarrow 0$ at other pressure values of the described region up to 27 kbar, only the corresponding anomaly of optical functions will be shifted to higher values of pressure.

It was shown [4–9,12] that the structural parameters such as the hydrogen bond length ($2R$), the distance between two proton-sites on a hydrogen bond (δ) and the rotation angle of PO₄-groups around the c -axis (θ) vary linearly with pressure in a pressure region from 1 bar to 17 kbar: $\Delta\theta/\Delta p = 5.8 \cdot 10^{-2} \text{ degree/kbar}$, $\Delta(2R)/\Delta p = -1.8 \cdot 10^{-3} \text{ \AA/kbar}$, $\Delta(\delta)/\Delta p = -3.2 \cdot 10^{-3} \text{ \AA/kbar}$. For the lattice parameters a and c we have: $\Delta c/\Delta p = -7.152 \cdot 10^{-3} \text{ \AA/kbar}$, $(\Delta a/\Delta p) \approx -7.46 \cdot 10^{-3} \text{ \AA/kbar}$. Some of these parameters ($2R, \theta, a, c$) continue to vary linearly at pressures up to 27 kbar [12].

There are anomalous changes of some structural parameters at $p = 27 \text{ kbar}$. The bond length decreases almost linearly with the increase of pressure, but at pressure values larger than 27 kbar it becomes much longer. The rotation angle θ increases abruptly at 27 kbar, too. These changes are probably connected with the softening of PO₄ groups, which was observed experimentally at pressure values $p > 27 \text{ kbar}$ [12].

In this work we have investigated an electron band structure of the KDP-type crystals as a function of the external hydrostatic pressure. We have used the

experimental data on the structural changes induced by pressure. The joint density of electron states, real and imaginary parts of the dielectric permeability, refraction indices, absorption and reflection coefficients for different polarizations of light are determined. Their pressure and frequency dependencies are investigated.

There are no other band structure calculations in the literature to compare with, and the dielectric response has not been studied by other authors at frequencies which correspond to the energies of electron transitions. Up till now, calculations of separated groups H_nPO_4 ($n=0,1,\dots,4$) electronic spectra have been presented [13,14,15]. The obtained [14,15] spectra were used to calculate the contribution of H_nPO_4 groups to the refractive index and the gyration effect.

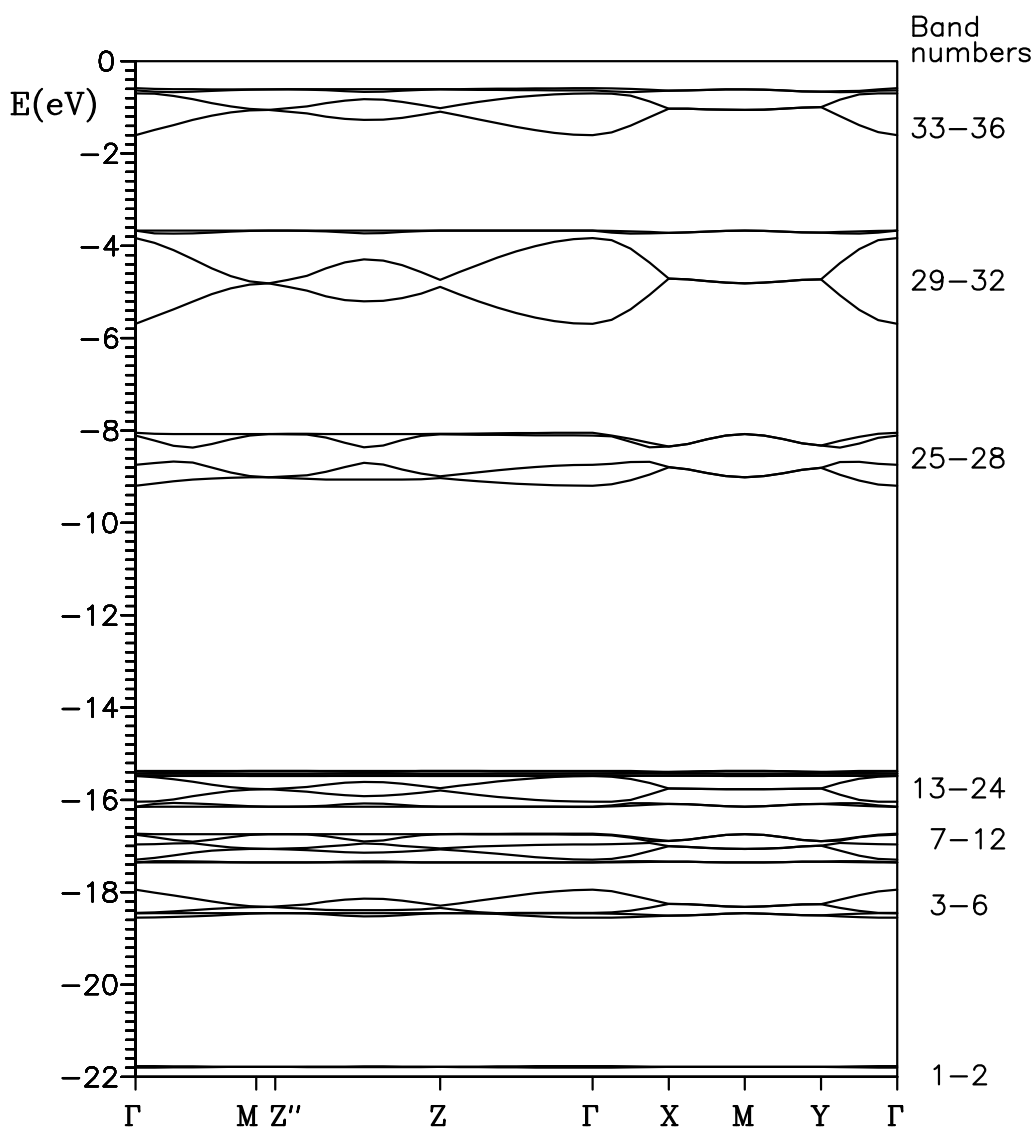


Figure 1. Electron band spectrum for a KH_2PO_4 crystal.

Table 1. The values of the electron energies (in eV) at Γ , M and X points of the Brillouin zone for the upper occupied band (number 24) and a set of the low-lying empty bands (numbers 25–31) at various values of pressure.

p (kbar)	band number							
	31	30	29	28	27	26	25	24
	Γ -point							
0.001	-3.6716	-3.8348	-5.6901	-8.0494	-8.1058	-8.7409	-9.1949	-15.3636
17.0-0.0	-3.6716	-3.8169	-5.7026	-8.0140	-8.0651	-8.6080	-9.0769	-15.3636
17.0+0.0	-3.6716	-3.7744	-5.7351	-8.0439	-8.0439	-8.5816	-9.0695	-15.3636
	M-point							
0.001	-3.6716	-4.8128	-4.8128	-8.0777	-8.0777	-9.0109	-9.0109	-15.3636
17.0-0.0	-3.6716	-4.8062	-4.8062	-8.0396	-8.0396	-8.8892	-8.8892	-15.3636
17.0+0.0	-3.6716	-4.8078	-4.8078	-8.0439	-8.0439	-8.8759	-8.8759	-15.3636
	X-point							
0.001	-3.7167	-4.7119	-4.7120	-8.3453	-8.3453	-8.7931	-8.7932	-15.3732
17.0-0.0	-3.7193	-4.7240	-4.7243	-8.2817	-8.2817	-8.6884	-8.6885	-15.3732
17.0+0.0	-3.7223	-4.7267	-4.7270	-8.3057	-8.3058	-8.6543	-8.6545	-15.3732

2. Band electron spectrum of the KH_2PO_4 crystal

The electron energy spectrum of the KDP-type crystals is calculated using the tight-binding approximation. The electron wave functions are presented as linear combinations of the Bloch functions which were constructed from the 3s and 3p orbitals of phosphorus, 2p oxygen and 1s hydrogen orbitals:

$$\psi_{\vec{q}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{nks} e^{i\vec{q}\vec{R}_{nk}} \cdot C_{ks}(\vec{q}) \cdot \varphi_{nks}(\vec{r} - \vec{R}_{nk}). \quad (2.1)$$

Here n is a unit cell number, k denotes an ion type and s is an index of electron states. The atomic orbitals φ_{nks} were chosen in the form of Slater functions. A set of linear equations for the expansion coefficients $C_{ks}(\vec{q})$ is obtained from the solution of the Schrödinger equation with wave functions (2.1) using an extended Huckel method (see [16]):

$$\sum_{ks} [\tilde{H}_{k's',ks}(\vec{q}) - E(\vec{q}) \cdot \tilde{S}_{k's',ks}(\vec{q})] \cdot C_{ks}(\vec{q}) = 0. \quad (2.2)$$

Secular equations (2.3) provide a band energy spectrum

$$|\tilde{H}_{k's',ks}(\vec{q}) - E(\vec{q}) \cdot \tilde{S}_{k's',ks}(\vec{q})| = 0, \quad (2.3)$$

where

$$\tilde{S}_{k's',ks}(\vec{q}) = \sum_n S_{n'k's',nks} \cdot e^{i\vec{q}(\vec{R}_{nk} - \vec{R}_{n'k'})}, \quad (2.4)$$

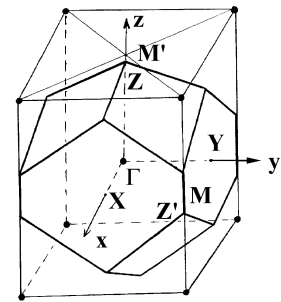


Figure 2. The first Brillouin zone for a KH_2PO_4 crystal. The line ZM' is equivalent to the $Z'M$ line.

$$\tilde{H}_{k's',ks}(\vec{q}) = \sum_n H_{n'k's',nks} \cdot e^{i\vec{q}(\vec{R}_{nk} - \vec{R}_{n'k'})}, \quad (2.5)$$

$$S_{n'k's',nks} = \int \varphi_{n'k's'}(\vec{r} - \vec{R}_{n'k'}) \cdot \varphi_{nks}(\vec{r} - \vec{R}_{nk}) dV, \quad (2.6)$$

$$H_{n'k's',nks} = \int \varphi_{n'k's'}(\vec{r} - \vec{R}_{n'k'}) \cdot \hat{H} \varphi_{nks}(\vec{r} - \vec{R}_{nk}) dV, \quad (2.7)$$

The summation in equations (2.4) and (2.5) was done over the nearest neighbours only. Secular equation (2.3) of the 36th order with complex matrix elements was solved for the arbitrary wave vector \vec{q} . Here we take into account the structure changes induced by the external hydrostatic pressure. The dependence of the R_{O-H} distance as well as the rotation angle of PO_4 -groups around the c-axis on pressure results in a pressure dependence of overlap integrals (2.6) and matrix elements of the Hamiltonian (2.7) and, thus, the band electron spectrum becomes a function of the external hydrostatic pressure. The calculations of the overlap integrals (2.6) and the matrix elements (2.7) are described in detail in our previous paper (see [16]). The results of the band structure calculation at the atmospheric pressure ($p \approx 1$ bar) for \vec{q} directed along the principal directions of the first Brillouin zone (BZ) are shown in figure 1. The dependence of the electron spectrum on pressure at Γ , M and X-points in BZ is presented in table 1. The first BZ for a KH_2PO_4 crystal is shown in figure 2. The state numbers are classified according to energy values. The bands from (1) up to (24) are filled in the ground state. The obtained energy gap is 6.17 eV, which is somewhat less than the experimental results: 7.0 eV [17], 7.62 eV [18].

The most essential changes under the influence of hydrostatic pressure are observed for the electron energy bands which are formed mostly by 1s-orbitals of hydrogen atoms (their numbers are 25–28). There are groups of bands which do not change with pressure (numbers 1,2; 7,8; 13,14; 31,32). We can include in these groups the upper occupied bands (numbers 17–24) the changes of which are smaller than $2 \cdot 10^{-3}$ eV, with the pressure change from 1 bar to 18 kbar. The dependence on the wave vector \vec{q} for these bands is very weak. The widths of these bands are less than $2 \cdot 10^{-2}$ eV, except for numbers 13, 14, 31, 32 which are of the order $4 \cdot 10^{-2} \div 1 \cdot 10^{-1}$ eV. It should be noted that at $q=0$ the energy values for the majority of these bands coincide with the energies of the corresponding levels (2B, 4A, 4B, 8B) of a separate group $H_2PO_4^-$ with the point symmetry C_2 , up to $1 \cdot 10^{-3}$ eV [14].

3. Optical properties

The imaginary part of dielectric susceptibility was calculated from the following relation [19]:

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{m^2 \omega^2} \sum_{i,j} \int \frac{2d\vec{q}}{(2\pi)^3} |\vec{e} d_{ij}(\vec{q})|^2 \delta(E_i(\vec{q}) - E_j(\vec{q}) - \hbar\omega), \quad (3.1)$$

Table 2. The calculated values of the piezooptic coefficients for a KH_2PO_4 crystal for various lengths of a light wave (in $10^{-13} \text{ cm}^2/\text{dyn}$).

λ (nm)	400	500	600	800	1000	1200
dn_o/dp	14.4	14.3	14.0	14.0	14.0	14.0
dn_e/dp	15.0	15.0	15.0	15.0	15.0	15.0
$d\varepsilon_{xx}^{-1}/d\sigma$	7.39	7.69	7.71	7.90	7.97	8.02
$d\varepsilon_{zz}^{-1}/d\sigma$	7.50	7.89	8.10	8.32	8.40	8.45

where

$$\vec{e} \cdot \vec{d}_{ij}(\vec{q}) = \langle \psi_{i\vec{q}} | \vec{e} \cdot \vec{p} | \psi_{j\vec{q}} \rangle = \vec{e} \cdot \int \psi_i^*(\vec{q}, \vec{r}) (-i\hbar\nabla) \cdot \psi_j(\vec{q}, \vec{r}) d\vec{r}. \quad (3.2)$$

The indices j and i denote the occupied and empty bands, respectively, and \vec{e} is a unit vector of the polarization of light. Integration in equation (3.1) is performed over the first BZ. The real part of the dielectric susceptibility ε_1 for all frequencies is determined by the Kramers-Kronig dispersion relation:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \omega' \varepsilon_2(\omega') \frac{1}{\omega'^2 - \omega^2} d\omega'. \quad (3.3)$$

Besides that, ε_1 within the transparency region was also calculated from the following relation [19]:

$$\varepsilon_1(\omega) = 1 + \frac{8\pi^2 e^2 \hbar^2}{m^2} \sum_{i,j} \int \frac{2d\vec{q}}{(2\pi)^3} \cdot \frac{|\vec{e} \vec{d}_{ij}(\vec{q})|^2}{[E_i(\vec{q}) - E_j(\vec{q})]} \cdot \frac{1}{[E_i(\vec{q}) - E_j(\vec{q})]^2 - (\hbar\omega)^2}. \quad (3.4)$$

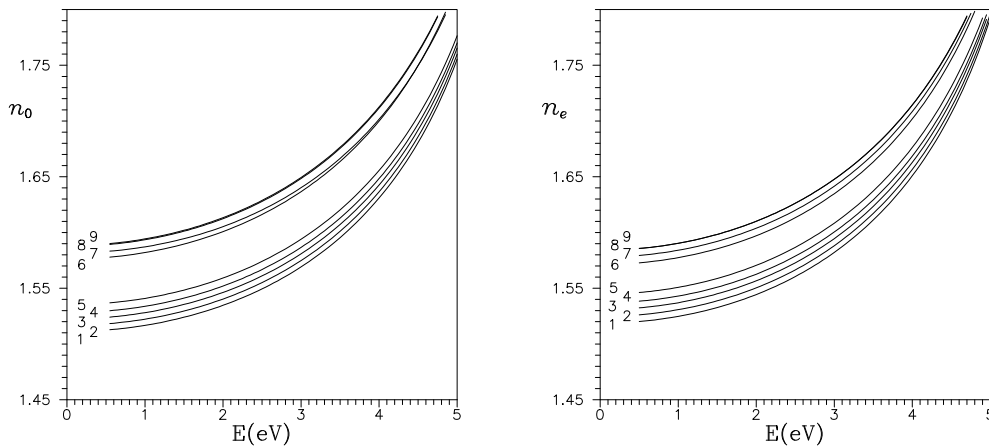


Figure 3. Spectral dependencies of the refractive indices n_o and n_e for KH_2PO_4 for various values of hydrostatic pressure: 1 – 1 bar, 2 – 4 kbar, 3 – 8 kbar, 4 – 12 kbar, 5 – (17.0 - 0.0) kbar, 6 – (17.0+0.0) kbar, 7 – 22 kbar, 8 – (27.0 - 0.0) kbar, 9 – (27.0 + 0.0) kbar.

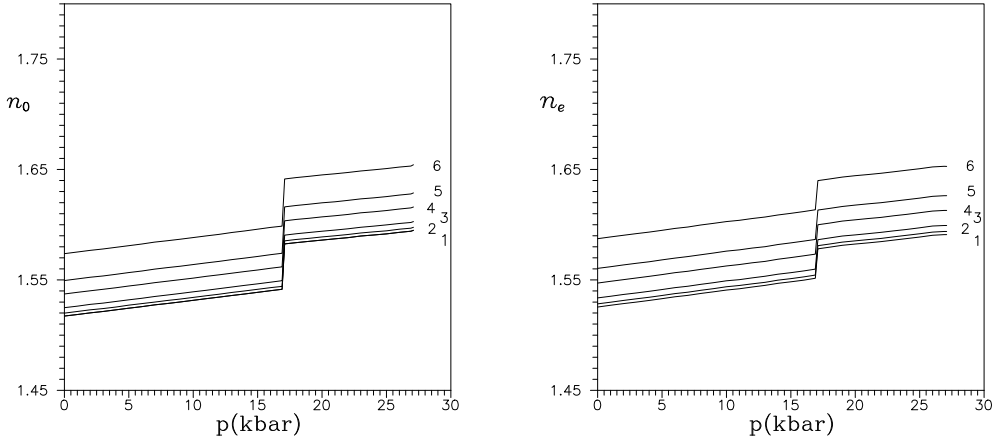


Figure 4. The pressure dependence of the refraction indices n_o and n_e for KH_2PO_4 for various lengths of a light wave: 1 – 1200 nm, 2 – 1000 nm, 3 – 800 nm, 4 – 600 nm, 5 – 500 nm, 6 – 400 nm.

The optical activity of crystals (i.e. gyrotropy) is a particular manifestation of spatial dispersion and is described by the linear term in the expansion of the dielectric permeability tensor $\varepsilon_{\alpha\beta}$ in powers of wave vector \vec{q} [20]:

$$\varepsilon_{\alpha\beta}(\omega, \vec{q}) = \varepsilon_{\alpha\beta}^{(0)}(\omega) + i \sum_{\gamma} A_{\alpha\beta,\gamma}^{(1)}(\omega) \cdot q_{\gamma} + \dots \quad (3.5)$$

We have calculated $g_{11} = \frac{\omega}{c} A_{yz,x}^{(1)}$ – a component of the gyration tensor, using the relation

$$A_{\alpha\beta,\gamma}^{(1)}(\omega) = -8\pi\hbar c \sum_{i,j} \int \frac{2d\vec{q}}{(2\pi)^3} \cdot \frac{\text{Im}[d_{ji}^{\alpha}(\vec{q})m_{ij}^{\beta\gamma}(\vec{q}) + m_{ji}^{\alpha\gamma}(\vec{q})d_{ij}^{\beta}(\vec{q})]}{[E_i(\vec{q}) - E_j(\vec{q})]^2 - (\hbar\omega)^2}, \quad (3.6)$$

where

$$m_{ij}^{\beta\gamma} = \langle \psi_{i\vec{q}} | \hat{m} | \psi_{j\vec{q}} \rangle = \int \psi_i^*(\vec{q}, \vec{r}) (r^{\gamma} p^{\beta} - r^{\beta} p^{\gamma}) \cdot \psi_j(\vec{q}, \vec{r}) d\vec{r}. \quad (3.7)$$

The joint density of electron states is given by [19]:

$$J_{ij}(\omega) = \int \frac{2d\vec{q}}{(2\pi)^3} \delta[E_i(\vec{q}) - E_j(\vec{q}) - \hbar\omega]. \quad (3.8)$$

It provides the density of the pairs of states; one of them is occupied and the other is vacant, their energies differ by $\hbar\omega$.

The integrals in equations (3.1), (3.4), (3.6), (3.8) were replaced by the sums over points \vec{q} in the first BZ. We included 1836 points in the BZ, then the accuracy of the results is within 10%. At each \vec{q} point, the band spectrum $E(\vec{q})$ and matrix elements of the electric $e\hat{d}$ and magnetic $\frac{e}{2mc}\hat{m}$ dipole electron momenta, defined by equations (3.2) and (3.7), respectively, were calculated. The values of $\varepsilon_1(\omega)$ obtained from equation (3.4) and from the Kramers-Kronig relation (3.3) differ by

less than 1%. For the calculation of ε_2 from equation (3.1) and in equation (3.8) we approximated the δ -function in the following way:

$$\delta[E_i(\vec{q}) - E_j(\vec{q}) - \hbar\omega_0] = \begin{cases} 1/\Delta, & |E_i - E_j - \hbar\omega_0| \leq \Delta/2 \\ 0, & |E_i - E_j - \hbar\omega_0| > \Delta/2 \end{cases}, \quad (3.9)$$

where parameter Δ is taken equal to 0.05 eV. We calculated the values for refractive indices n , extinction coefficients K , absorption coefficients α and reflection R . The formulas presented below were used:

$$n = \sqrt{\frac{1}{2} \left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1 \right)}, \quad K = \sqrt{\frac{1}{2} \left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1 \right)},$$

$$\alpha(\omega) = \frac{2\omega}{c} \cdot K(\omega), \quad R = \frac{(n-1)^2 + K^2}{(n+1)^2 + K^2}. \quad (3.10)$$

We have found that the refractive indices n_0 and n_e change almost linearly with pressure in the pressure region 1 bar $\leq p < 17$ kbar. The calculated pressure and frequency dependencies of the optical constants are shown in figures 3–8. Their anomalous behaviour at the pressure values $p = 17$ kbar and $p = 27$ kbar are due to the changes of an electron spectrum and wave functions (see table 1) which are induced by the structure changes described above. The obtained changes of the optical constants at $p = 27$ kbar are less essential than at $p = 17$ kbar. It was taken into account that for pressure values above $p \simeq 17$ kbar the hydrogen bond is transformed from two-minimum to one-minimum bond, when the proton is localised at the midpoint of the hydrogen bond. The correlation between the character of a proton distribution and the

changes of n_0 , n_e and g_{11} is essential, so it is interesting to study experimentally the behaviour of optical constants with the pressure change in order to investigate their possible anomalies at high pressures ($p \geq 17$ kbar). Such investigations will give us a possibility to learn the behaviour of protons at high pressure and, thus, to examine the nature of the ferroelectric phase transition from a new point of view. The obtained dispersion of the refractive indices is stronger than the one observed experimentally (see figure 5). One can predict such results because we have obtained from the calculations the energy gap somewhat less than the experimental

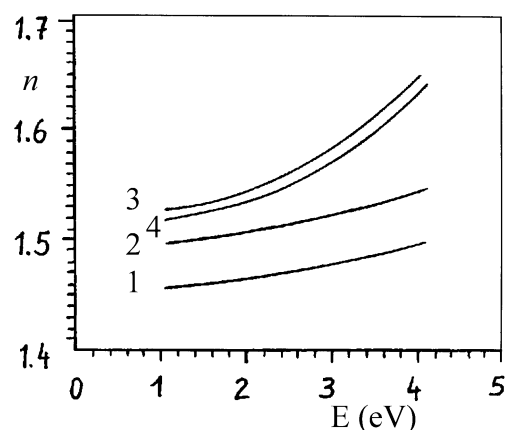


Figure 5. Spectral dependencies of the refraction indices for KH_2PO_4 at the atmospheric pressure ($p = 1$ bar). 1,2 – experimental data [22], 3,4 – calculated, 1,3 – n_e , 2,4 – n_o .

data (see above). It may be caused by the single-electron approximation used for band structure calculations. Besides, we did not use any fitting parameters in the calculation of the electron spectrum and optical constants.

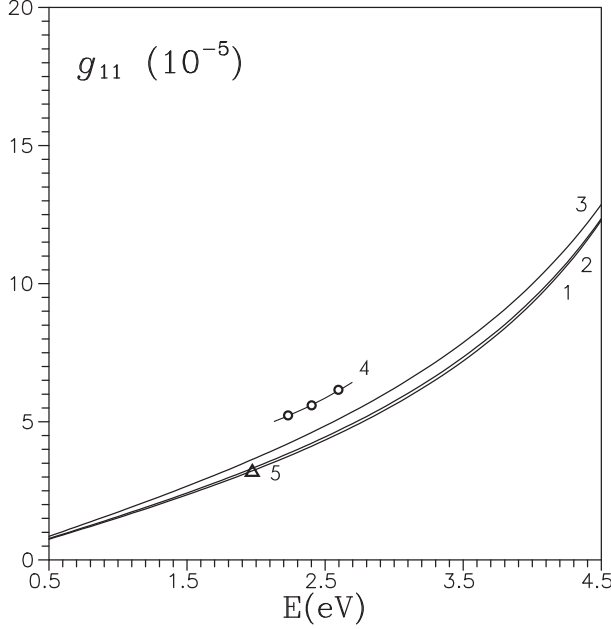


Figure 6. Spectral dependence of the g_{11} component of the gyration tensor for KH_2PO_4 for various values of hydrostatic pressure: 1 – 1 bar, 2 – (17.0 - 0.0) kbar, 3 – (17.0 + 0.0) kbar, 4 – 1 bar, 5 – 1 bar; 1,2,3 – calculated, 4,5 – experimental data [24], [25].

It is characteristic especially of the A maximum which lies in the frequency region $\hbar\omega \sim 9 - 10$ eV. That effect is more essential for the light polarized perpendicularly to the c -axis. The dependence of the optical functions which describe the absorption and reflection of the light polarized parallelly to the c -axis (functions K_3 , ε_2^{zz} etc) on pressure is less essential. The anomalous increase of functions K_1 , ε_2^{xx} at pressure passing the value $p \simeq 17$ kbar is larger than the increase of these functions when the pressure is changed from 1 bar to 17 kbar (see figure 7).

It is possible to determine piezoptic coefficients using the obtained pressure dependencies of the coefficients n_0 and n_e . In order to describe the change of the dielectric susceptibility $\varepsilon_{\alpha,\beta}$ with the pressure change we shall utilize the following relation:

$$\varepsilon_{\alpha\beta}^{-1}(\omega\sigma) = \varepsilon_{\alpha\beta}^{(0)-1}(\omega) + \sum_{ke} \pi_{ijk e} \sigma_{ke}, \quad (3.11)$$

where $\pi_{ijk e}$ are piezoptic coefficients, σ_{ke} is a tensor of mechanical strain.

The main features of the obtained absorption and reflection spectra at the atmospheric pressure ($p \approx 1$ bar) are in agreement with the experimental data [13, 17] (see figure 8). A wide absorption band at energies 8.5–10.0 eV corresponds to the **A** band in the experiment, while the absorption bands at 10.5–11.2 eV and 11.8–12.7 eV correspond to the **B** and **C** bands, respectively. A huge absorption band at 14.0–15.8 eV coincides with the **D** band obtained experimentally. It should be noted that we have obtained the absorption bands in the energy region 6–8 eV, which are not observed experimentally.

Let us consider in more detail the dependence of the absorption spectra on hydrostatic pressure. An increase of the main maxima of the absorption and reflection spectra with pressure takes place.

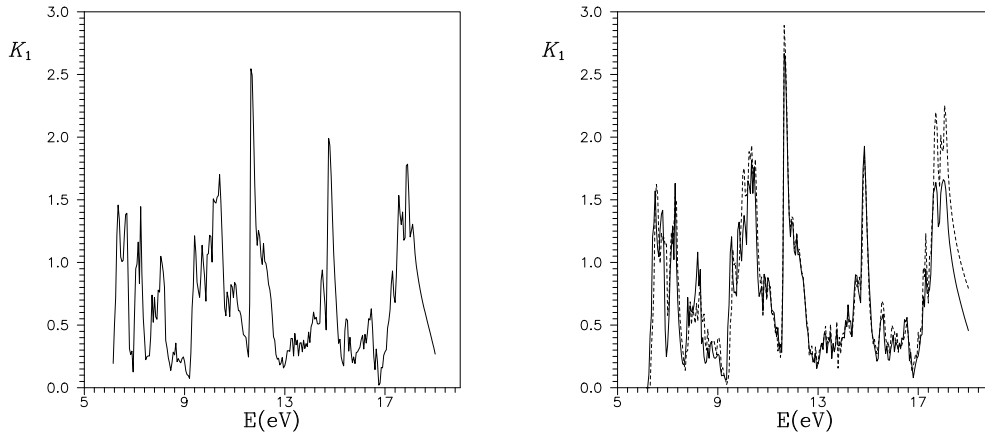


Figure 7. Spectral dependence of the extinction coefficient K_1 for the light polarized perpendicularly to the c -axis, for KH_2PO_4 at various values of hydrostatic pressure: (a) – 1 bar, (b) – (17.0 - 0.0) kbar – solid line, (17.0 + 0.0) kbar – dashed line.

In the case of a hydrostatic pressure we have:

$$\frac{d(\varepsilon_{xx}^{-1})}{d\sigma} = \pi_{11} + \pi_{12} + \pi_{13} \quad \frac{d(\varepsilon_{zz}^{-1})}{d\sigma} = \pi_{31} + \pi_{32} + \pi_{33} \quad (3.12)$$

We have found that the piezooptic coefficients $d(\varepsilon_{xx}^{-1})/d\sigma$ and $d(\varepsilon_{zz}^{-1})/d\sigma$ do not depend on pressure. Their changes with the change of pressure from 1 bar to 17 kbar at fixed frequency are less than 2.5%. The calculated values of the piezooptic coefficients are presented in table 2. On the other hand, using the experimental data for π_{ij} (for $\lambda = 632.8$) nm [21,22] we have: $d(\varepsilon_{xx}^{-1})/d\sigma = 9.35 \cdot 10^{-13} \text{ cm}^2/\text{dyn}$; $d(\varepsilon_{zz}^{-1})/d\sigma = 7.64 \cdot 10^{-13} \text{ cm}^2/\text{dyn}$. So, the obtained piezooptic coefficients are in agreement with the experimental data. The g_{11} component of the gyration tensor practically does not change with pressure, except for the anomalies at $p=17$ kbar, when g_{11} abruptly increases approximately by 10%. In the case of ionic contributions to the optical properties of a KH_2PO_4 crystal we also obtained earlier a weak increase of the g_{11} component of the gyration tensor with the pressure change from 1 bar to 17 kbar [23].

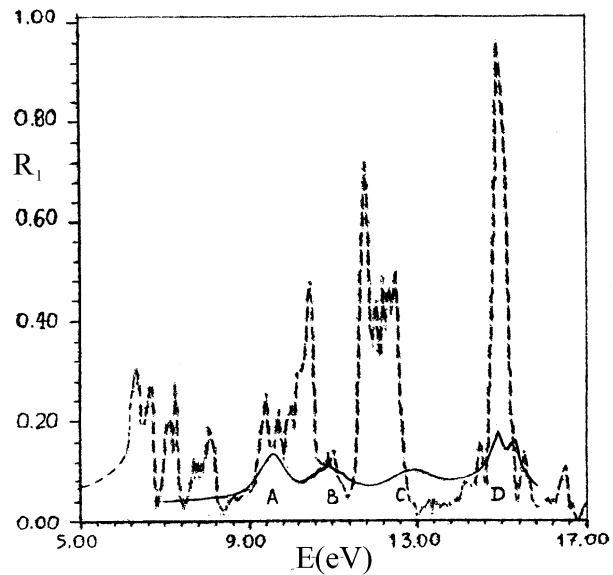


Figure 8. Spectral dependence of the reflection coefficient R_1 for KH_2PO_4 at the atmospheric pressure, solid line – experimental data [13], dashed line – calculated.

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Зонний електронний спектр і оптичні властивості кристалів типу KDP при наявності зовнішнього гідростатичного тиску

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В наближенні сильно зв'язаних електронів досліджено залежність зонного електронного спектру кристалів типу KDP від зовнішнього гідростатичного тиску. Розраховані комбінована густина електронних станів, дійсна та уявна частини діелектричної проникності для різної поляризації світла, показники заломлення, коефіцієнт гірації, коефіцієнти поглинання та відбивання світла. Досліджена їх залежність від енергії світлової хвилі та від зовнішнього гідростатичного тиску. Результати порівнюються з експериментальними даними для п'єзооптичних коефіцієнтів. Отримані аномалії оптичних констант при тиску $p \simeq 17$ кбар зумовлені трансформацією потенціалу протона на зв'язку з двомінімумного в одномінімумний.

Ключові слова: електронний спектр, гідростатичний тиск, оптичні властивості

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