KRISTOFEL', N. N. Cand Phys-Math Sci -- (diss) "Quantum-mechanical calculation of adiabatic potentials and certain properties of the centers of luminescence in alkali-haloid crystal phosphori." Tartu, 1959. 11 pp (Tartu State Univ), 225 copies (KL, 46-59, 135)

24(4), 24(2)

AUTHOR: Kristofel', N.N. SOV/51-7-1-11/27

TITLE: A Quantum-Mechanical Calculation of a Luminescence Centre in KCl-Tl. (Kvantovomekhanicheskiy raschet tsentra lyuminestsentsii v KCl-Tl)

PERIODICAL: Optika i spektroskopiya, 1959, Vol 7, Nr 1, pp 78-82 (USSR)

ABSTRACT: The author described earlier (Ref 1) a quantum-mechanical method of calculation of the adiabatic potentials of luminescence centres in alkali-halide crystal phosphors. Using this method the author discussed the $^1S_0$- and $^3P_1$ states of a luminescence centre in KCl-Tl (the results for the $^1S_0$- state were given in an earlier paper, Ref 2). The present paper reports results for the excited state and the spectral properties of such a centre. Each centre is assumed to consist of activator ions which replace one or more cations at a lattice site. The activator electrons are assumed to interact with local vibrations. The number of ions in one centre is equal to the number of ions taking part in interactions with local vibrations. It is also assumed that the activator ions interact only with fully symmetrical local vibrations. The adiabatic potentials of the $^1S_0$- and the $^3P_1$- states are shown as curves 1 and 2 in Fig 1. Fig 2 shows the empirical (dashed curve) and theoretical (continuous curve) spectra of a luminescence centre in KCl-Tl.

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A Quantum-Mechanical Calculation of a Luminescence Centre in KCl-Tl SOV/51-7-1-11/27

The empirical spectrum was taken from Ch.B. Lushchik et al (Ref 8). The theoretical spectrum, deduced from the luminescence centre model described above, agreed quite well with the empirical one. Other spectral properties of a luminescence centre (such as the emission and absorption half-widths) calculated by the author are given, together with corresponding experimental values (taken from Ref 7), in Table 3. For all these properties the agreement between theory and experiment is good and consequently the author concludes that the results obtained by him confirm the assumed model of a luminescence centre in KCl-Tl. The present paper will be published in an extended form in "Trudy IFA AN Estonskoy SSR". Acknowledgment is made to M.I. Petrashen' who directed and helped in this work and to K.K. Rebane and Ch.B. Lushchik for their advice. There are 2 figures, 3 tables and 14 references, 8 of which are Soviet and 6 English.

SUBMITTED: January 10, 1959

Card 2/2

23337 S/058/61/000/006/023/063
A001/A101

24.7100 (1142, 1153, 1160)

AUTHOR: Kristofel', N.N.

TITLE: The bond energy in TlCl crystals

PERIODICAL: Referativnyy zhurnal. Fizika, no. 6, 1961, 177-178, abstract 6V323 ("Tr. In-ta fiz. i astron. AN EstSSR". 1960, no. 1, 262 - 263)

TEXT: The author points out that the energy of "non-point" interactions, calculated earlier for the ion pair Tl^+ - Cl applied to KCl-Tl phosphor, can be used for quantum-mechanical calculations of the bond energy and lattice constant of the TlCl crystal. The following formula was obtained for the bond energy V (in atom. units): $V/N_A = -1.763/a + 8\,[0.0147 - 0.0309\,(a-5.944) + 0.0220\,(a-5.944)^2] - (2376/a^6 + 13710/a^8)$, where N_A is Avogadro number, a is separation between ions of Tl^+ and Cl^-. The first term represents Madelung's energy, the second term is the sum of an "electrostatical correction" for inaccuracy of ions, the exchange energy and S-energy which takes into account non-orthogonality of the ion wave functions. The last term corresponds to multipole interactions. As a result it was obtained: $a_0 = 3.40$ Å, V = - 171.5 kcal/mol, which correspond to experimental values equal to a = 3.33 Å (T = 20°C) and V = -170.9 kcal/mol.

[Abstracter's note: Complete translation]

N. Maksimova

Card 1/1

83923

9.4300 (1035,1138,1143)

S/051/60/009/004/023/034
E201/E191

AUTHORS: Petrashen', M.I., Abarenkov, I.V., and Kristofel',N.N.

TITLE: Approximate Wave-functions of Free Ions and of Ions in a Crystal

PERIODICAL: Optika i spektroskopiya, 1960, Vol 9, No 4, pp 527-529

TEXT: In quantum-mechanical calculations of properties of alkali-halide crystals, the one-electron functions of free ions are used as the functions of ions in a crystal. This approach is not very satisfactory. The present note describes a simple method of calculating approximate one-electron functions of a "central ion" (CI) in an ionic crystal. The one-electron functions of a free CI are assumed to be known. They are then modified by allowing for the effect of other ions in the lattice, regarded as geometrical points. The new functions are known as crystalline one-electron functions and they can be used in the zeroth approximation of the perturbation theory. The next step would be an allowance for the departure from the assumed point geometry of the lattice. The calculation method described here was tested by calculating diamagnetic susceptibility of a crystal.

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S/051/60/009/004/023/034
E201/E191

Approximate Wave-functions of Free Ions and of Ions in a Crystal

It was found that the results obtained with crystalline functions agreed better with experiment than the results deduced using free-ion functions. The paper is entirely theoretical.

There are 6 references: 4 Soviet, 1 English and 1 German.

SUBMITTED: April 16, 1960

Card 2/2

X

KRISTOFEL', N.N.

Interaction between the activator and in completely symmetrical local vibrations. Opt. i spektr. 9 no.5:615-620 N '60. (MIRA 13:11)

(Luminescence)

PETRASHEN', M.I.; ABARENKOV, I.V.; KRISTOFEL', N.N.

Approximate wave functions of free ions and ions in crystals. Vest. LGU 15 no.16:7-21 '60. (MIRA 13:8)
(Ions) (Wave mechanics)

KRISTOFEL', N.N.

Stability of structures of the cesium and sodium chloride type in TlCl crystals. Fiz. tver. tela 3 no.6:1876-1878 Je '61.
(MIRA 14:7)

1. Institut fiziki i astronomii AN Estonskoy SSR, Tartu.
(Thallium chloride crystals) (Cesium chloride crystals)
(Salt crystals)

ABARENKOV, I.V.; KRISTOFEL', N.N.; PETRASHEN, M.I.

Calculation of the optical properties of small-radius electron centers in ionic crystals. Opt. i spektr. 10 no.4:487-492 Ap '61.
(MIRA 14:3)

(Ionic crystals—Spectra)

S/058/62/000/008/042/134
A061/A101

AUTHOR: Kristofel', N. N.

TITLE: A contribution to the theory of excess valency impurities in ionic crystals

PERIODICAL: Referativnyy zhurnal, Fizika, no. 8, 1962, 42, abstract 8V293 ("Tr. In-ta fiz. i astron. AN EstSSR", 1961, no. 15, 3 - 20; summary in English)

TEXT: The quantum-mechanical method of calculating the properties of impurity centers in ionic crystals is generalized to the case of impurities of anomalous valency. Energy corrections of the ion-multipole type are absent when use is made of ionic wave functions, and the deforming effect of the point lattice field is taken into account. The said corrections occur in the case of impurities of anomalous valency. Calculations are made for the formation energies, the shifts of equilibrium positions, and the frequencies of local vibrations for the cationic and anionic vacancies in KCl. A quasioptical local vibration develops here. The ground state of a center due to a Ge^{2+} ion building

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in the KCl cationic lattice point is calculated, and some characteristic features of such centers are discussed.

[Abstracter's note: Complete translation]

S/613/61/000/017/001/011
D051/D113

AUTHOR: Kristoffel, N.N.

TITLE: The effect of the type of host crystal structure on the spectral characteristics of phosphors

SOURCE: Akademiya nauk Estonskoy SSR. Institut fiziki i astronomii. Trudy, no. 17, 1961. Issledovaniya po lyuminestsentsii, 3-28

TEXT: Since the effect of the type of host crystal structure on the spectral characteristics of phosphors with built-in activators is insufficiently studied, the phosphor KCl-Tl in the structural form of a CsCl crystal was investigated. The quantum-mechanical method of calculating the adiabatic potentials of centers of luminescence, which had previously been used for a phosphor with an NaCl host crystal, was used in this case. The result of a calculation for KCl-Tl based on single-oscillation approximation, did not convey the changes observed in the spectra of this phosphor; the maxima of the spectral bands shift in the opposite direction. The Jahn-Teller effect

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Card 1/2

S/613/61/000/017/001/011
D051/D113

The effect of the type ...

was examined for the center of luminescence in a host crystal of the CsCl type. The adiabatic potential minima correspond to the nuclear configurations of symmetry D_{3h} and D_{2h}, the D_{3h} minima being equilibrium potentials. The difference in the corresponding spectral effects for centers of both structures allows them to be identified. There are 7 figures and 3 tables.

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Card 2/2

22188
S/048/61/025/004/037/048
B117/B212

24.3500 (1138,1137,1395)

AUTHOR: Kristofel', N. N.

TITLE: Interaction between an activator and not completely symmetric local vibrations

PERIODICAL: Izvestiya Akademii nauk SSSR. Seriya fizicheskaya, v. 25, no. 4, 1961, 533-535

TEXT: The present paper was read at the 9th Conference on Luminescence (crystal phosphors). The author has used the theory of perturbation to calculate the interaction of an activator with not completely symmetric vibrations. Concrete calculations have been made for the $^3P_1$ term of the center in KCl-Tl. Only shifts of neighboring activators have been taken into account. The frequencies of local vibrations have been calculated with a method described earlier (Ref. 1: Tr. In-ta fiz. i astron. EstSSR, no. 10, 3 (1959)). In contradiction to "longitudinal" vibrations the frequencies of "transverse" vibrations will be increased during excitation of Tl^+. It has been shown that symmetric vibrations (normal coordinates

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S/048/61/025/004/037/048
B117/B212

Interaction between an...

y_1 and y_2) will lead to a minimum of the adiabatic potential and the symmetry of the center will decrease to D_{4h}. There are three similar configurations for balanced conditions which differ in the direction of the symmetrical axis of 4th order. the "dumbbell" of the 6p-function of the Tl^+ is orientated along it. Cl-ions move away on this axis from Tl^+ by 0.110 A, and they approach it normally by 0.055 A. In steady-state configurations there is a non-abnormal and a doubly abnormal level with relative energies of 0.065 resp. 0.13 ev. This splitting up is lesser than that of a multiplet. At the point $y_1 = y_2 = 0$, it corresponds to the steady-state configuration of the ground state, all three "leaves" have the same, i.e., zero value. Centers with big radius interacting with crystal vibrations do not seem to have the Jahn-Teller effect. The calculated results make it possible to explain the low temperature polarization of the $^3P_1 \longrightarrow {}^1S_0$ radiation in KCl-Tl as found in Ref. 4 (C. Klick, W. Compton, J. Phys. Chem. Solids, 7, 170 (1958)) and assign to it a vibrational character. Due to the Jahn-Teller effect the emission

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B117/B212

Interaction between an...

bands might be non-elementary under certain conditions and even show a splitting in the absorption spectrum. By using the adiabatic potentials of the single-oscillator approximation (in ev and A): $I(^1S_0) = 18.0(q - 0.093)^2$, $I(^3P_1) = 4.34 + 11.4(q + 0.065)^2$ (Ref. 1) and the results of this paper the spectral characteristics of $^1S_0 \longleftrightarrow {}^3P_1$ bands in KCl-Tl have been calculated by taking into account the not completely symmetric vibrations (Table: in ev). These contribute ~18% to Stokes' losses $(E_m^{x} - E_m^{I})$ and δ ~10% to the half-width. The activator will react much stronger with not completely symmetric vibrations in alkali halide phosphors. This explains the relatively good applicability of the single-oscillator approximation. If a uniform compression is investigated, the not completely symmetric vibrations are not essential in a quasi-molecular model if this effect does not bring about a change of steady-state values of corresponding vibration coordinates. S. A. Moskalenko has stated the following in a discussion about this paper: A localized center will not change the symmetry of the lattice and the interaction will take place with vibrations having the wave vector $\vec{k} = 0$. Therefore, a decrease of

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Interaction between an...

S/048/61/025/004/037/048
B117/B212

the symmetry must not necessarily take place in this problem and the splitting of the center level cannot be understood. It could be understood if it would be due to the interaction with lattice vibrations having the wave vector $\vec{k} \neq 0$. K. K. Rebane has said to the same paper: The symmetry considerations seem to be correct. But the applicability of the quasi-molecular model is not proven. There are 1 table and 6 references: 2 Soviet-bloc and 4 non-Soviet-bloc.

ASSOCIATION: Institut fiziki i astronomii Akademii nauk EstSSR (Institute of Physics and Astronomy of the Academy of Sciences Estonskaya SSR)

Legend to the table:
1) Single-oscillator approximation; 2) having taken into account the not completely symmetrical vibrations;
3) experiment.

	E_m^{κ}	E_m^{l}	$E_m^{\kappa}-E_m^{l}$	δ_{κ}	δ_{l}
1) Одноосцилляторное приближение	4,64	3,90	0,74	0,23	0,45
2) С учетом неполносимметричных колебаний	4,66	3,76	0,90	0,25	0,50
3) Эксперимент	5,02	4,06	0,96	0,23	0,51

Card 4/4

TOLPYGO, K.B.; KRISTOFFEL, N., red.

[Theory of vibrations of crystal lattices with deformed atoms] Teorii kolebanii kristallicheskikh reshetok s deformiruemymi atomami; lektsii, prochitannye v letnei shkole po teorii tverdogo tela. Tartu-Tyravere, iiun' 1961. Tartuskii gos. unov. Vol.2. 1962. 57 p. (MIRA 16:4)
(Crystal lattices--Vibration) (Dislocation in crystals)

S/181/62/004/001/008/052
B102/B138

AUTHOR: Kristofel', N. N.

TITLE: Theory of vibrations of a lattice with defects

PERIODICAL: Fizika tverdogo tela, v. 4, no. 1, 1962, 52 - 58

TEXT: A monatomic chain consisting of N+1 atoms (N is even) is considered, containing an impurity atom in its central site (n=0) and anchored at its ends. Neighboring chain links are assumed to interact quasielastically. The constant of the binding forces of the chain atoms is denoted by k, that between impurity and chain atoms by γ. The mass difference between impurity and chain atoms is neglected. x_n is the displacement of atoms in an ideal chain, being the distance to their equilibrium position $x_n^{(o)}$ is their displacement caused by the introduction of an impurity. The chain is assumed to maintain its length when the impurity is introduced, their end atoms have the positions n = ±N/2. Then

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Theory of vibrations of a...

S/181/62/004/001/008/052
B102/B138

$$\begin{cases} x_n^{(0)} = -\frac{D}{k}\left[1+P\left(\frac{N}{2}-1\right)\right]^{-1}\left(\frac{N}{2}-n\right) & (n>0), \\ x_0^{(0)} = 0, & \\ x_n^{(0)} = \frac{D}{k}\left[1+P\left(\frac{N}{2}-1\right)\right]^{-1}\left(\frac{N}{2}-|n|\right) & (n<0). \end{cases} \quad (4)$$

holds, and, with $q_n = x_n - x_n^{(0)}$, the equations of motion

$$\begin{cases} \frac{m}{\gamma}\ddot{q}_0 = q_1 + q_{-1} - 2q_0, \\ \frac{m}{k}\ddot{q}_1 = Pq_0 + q_2 - (1+P)q_1, \\ \frac{m}{k}\ddot{q}_{-1} = Pq_0 + q_{-2} - (1+P)q_{-1}, \\ \frac{m}{k}\ddot{q}_n = q_{n+1} + q_{n-1} - 2q_n \left(n \neq 0, \pm 1, \pm\frac{N}{2}\right). \end{cases} \quad (6)$$

are valid for the case of even vibrations. This set can be reduced to

$$\begin{cases} \frac{m}{k}\ddot{q}_1 = q_2 - (1+P)q_1, \\ \frac{m}{k}\ddot{q}_n = q_{n+1} + q_{n-1} - 2q_n \ \left(n \neq 0, 1, \frac{N}{2}\right). \end{cases} \quad (9),$$

the solution is given by

$$\begin{cases} q_n^{(s)} = Ae^{i\omega_s t}[\sin n\varphi_s + (P-1)\sin(n-1)\varphi_s] & (n \geqslant 1), \\ q_n^{(s)} = Ae^{i\omega_s t}[\sin n\varphi_s - (P-1)\sin(|n|-1)\varphi_s] & (n \leqslant -1) \end{cases} \quad (10)$$

$P = \gamma/k$, the frequencies are given by $\omega_s^2 = \frac{2k}{m}(1-\cos\varphi_s)$, $\sin \frac{N}{2}\varphi_s = (1-P)\sin(N/2-1)\varphi_s$. The latter equation has N real solutions in $0 \leqslant \varphi_s \leqslant \pi$, if $P > P_k$; $P_k = (1-1/N)(1/2-1/N)^{-1}$; the local vibration is described by $\varphi_L = \pi + i\varkappa$, its frequency $\omega_L^2 = \frac{2k}{m}(1+\text{ch}\,\varkappa)$. $\varkappa$ increases with P and at $P = P_k$, ω_L coincides with the ceiling of the band. If $P < 1$, no local vibrations occur. The local vibrations which are described by

$$\begin{cases} q_{nL} = Ae^{i\omega_L t}(-1)^n[\text{sh}\, n\varkappa + (1-P)\,\text{sh}(n-1)\varkappa] & (n > 0), \\ q_{nL} = Ae^{i\omega_L t}(-1)^n[\text{sh}\, n\varkappa - (1-P)\,\text{sh}(|n|-1)\varkappa] & (n < 0). \end{cases} \quad (15)$$

can be reduced to $q_n \approx A \frac{n}{|n|} e^{i\omega_L t}(1-P)^{-|n|}$, $\omega_L^2 = \frac{k}{m}\frac{P^2}{P-1}$. In an appendix

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Theory of vibrations of a...

S/181/62/004/001/008/052
B102/B138

the main equations for the odd harmonics are given. The author thanks I. V. Abarenkov for discussions and M. I. Petrashen' and K. K. Rebane for remarks. There are 2 figures and 19 references: 2 Soviet and 17 non-Soviet. The four most recent references to English-language publications read as follows: J. Mahanty, A. Maradudin, G. Weiss. Progr. Theor. Phys., 20, 369, 1958; E. Teramoto, S. Takeno. Progr. Theor. Phys., 24, 1349, 1960; R. Wallis, A. Maradudin. Progr. Theor. Phys., 24, 1055, 1960; B. Gourary, A. Maradudin. J. Phys. Chem. Solids, 13, 88, 1960.

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ASSOCIATION: Institut fiziki i astronomii AN ESSR Tartu (Institute of Physics and Astronomy AS Estonskaya SSR, Tartu)

SUBMITTED: July 7, 1961

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S/051/62/013/002/005/014
E032/E514

AUTHORS: Zavt, G.S. and Kristofel', N.N.

TITLE: On the applicability of the Condon approximation to a luminescence centre

PERIODICAL: Optika i spektroskopiya, v.13, no.2, 1962, 229-234

TEXT: The authors report the results of a calculation of the dependence of the electronic matrix element M(R) for the $^1S_0 \rightarrow {}^3P_1$ transition in the luminescence centre of the crystal phosphor KCl-Tl. The calculation is based on the model of the luminescence centre of the associated theory which was given in the previous papers by the second of the present authors (Tr.IFA AN ESSR, No.7, 85, 1958. Mater. VII soveshchenaiya po lyuminests., 49, Tartu, 1959; Tr. IFA AN ESSR, No.10, 3, 1959; No.11, 180, 1960; Opt. i spektr., 7, 78, 1959; Opt. i spektr., 10, 487, 1961). In an ionic crystal electron densities of the various ions overlap and hence the wave functions for the activator do not take the form of the wave functions of the free activator simply perturbed by the crystal field. They do in fact contain an admixture of wave functions due to the base ions.

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On the applicability of.... S/051/62/013/002/005/014
E032/E514

This effect is very dependent on the interionic distance and varies during the ion vibration process so that the electronic matrix elements depends on the nuclear coordinates $\underline{R}$. A consideration of the numerical results of these calculations leads to the conclusion that the Condon approximation is very adequate for the $^1S_0 \rightarrow {}^3P_1$ transition in KCl-Tl. There are 3 tables.

SUBMITTED: June 1, 1961

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Card 2/2

S/613/62/000/018/013/013
E039/E120

AUTHOR: Kristofel', N.N.

TITLE: On the possibility of discovering local vibrations in the Raman spectra of crystals

SOURCE: Akademiya nauk Estonskoy SSR. Institut fiziki i astronomii. Trudy. no.18. 1962. Issledovaniya po lyuminestsentsii. 149-152

TEXT: Only local vibrations of U-centres have to date been observed in the infrared spectra of some alkali halide crystals. The Raman spectra of crystal phosphors are of special interest as they must display local vibrations corresponding to interactions with electron defects in optical electron vibration transitions. The intensity of Raman spectra for local vibrations is much less intense than that of the first order spectra of such crystals. Hence crystals in which the first order is absent (the alkali halides) are investigated with the aim of discovering the first order peaks from local vibrations on the background of the continuous second order spectra. Frequencies connected with

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On the possibility of discovering ... S/613/62/000/018/013/013
E039/E120

anion and cation vacancies for KCl, NaCl and NaF are 3.91, 2.53 and 3.83 x 10^{13} sec^{-1} for anions, and 3.20, 3.22 and 3.83 x x 10^{13} sec^{-1} for cations, respectively. The frequency of local vibrations about F centres is larger than about anion vacancies. For example, a frequency of 4.08 x 10^{13} sec^{-1} is obtained for F centres in NaCl. For a more detailed elucidation of the question it is necessary to study the effect of changing the number of defects (vacancies) on separate parts of the Raman spectra.

SUBMITTED: March 2, 1962

Card 2/2

KRISTOFEL, N.N.; ZAVT, G.S.

International Congress on Lattice Dynamics, Copenhagen, Denmark
5-9 Aug '63

Institut de Physique et d'Astronomie de l'Academie des Sciences de
la R.S.S. d'Estonie, Tartu Observatoire, Tartu, U.S.S.R.

Title of Report-- Einige Fragen der Theorie von Schwingungen in Fremdionenent-haltenden ionenkristellen.

L-11155-63 EWT(1)/BDS--AFFTC/ASD

ACCESSION NR: AP3000600 S/0181/63/005/005/1279/1285

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51

AUTHOR: Kristofel', N. N; Zavt, G. S.

TITLE: The Condon approximation and the optical properties of impurity centers 21

SOURCE: Fizika tverdogo tela, v. 5, no. 5, 1963, 1279-1285

TOPIC TAGS: impurity centers, Jahn-Teller effect, Condon approximation, absorption bands

ABSTRACT: The authors discuss spectral phenomena resulting from the breakdown of the Condon approximation: the dependence of the integral spectrum on temperature and the appearance of spectral bands "forbidden" in a rigid lattice. They investigate the symmetry of vibrations that cause breakdown of the Condon approximation and "permit" nonadiabatic transitions, using as an example the transition sup 1 S sub 0 to sup 3 P sub 1 in KCl-Tl. They show that under certain conditions of splitting the adiabatic potential the consequences of the Jahn-Teller effect, as a result of breakdown of the Condon approximation, may lead to splitting of the absorption band. This follows from Equation (1). The authors conclude that breakdown of the Condon approximation, the Jahn-Teller effect, and the nonadiabatic behavior should be considered as related phenomena in the theory of optical properties of impurity centers. With this in mind they think it possible to predict new effects, the

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L 11155-63
ACCESSION NR: AP3000600

experimental discovery of which may be possibly brought about by microwave techniques. Orig. art. has: 12 formulas.

ASSOCIATION: Institut fiziki i astronomii AN EstSSR, Tartu (Institute of Physics and Astronomy AN EstSSR)

SUBMITTED: 16Nov62 DATE ACQ: 11Jun63 ENCL: 01

SUB CODE: PH NO REF SOV: 007 OTHER: 006

Card 2/3

KRISTOFFEL, N.N.; REBANE, K.K.

Some problems of the theory of luminescent centers in crystalline phosphors. Chekhosl fiz zhurnal 13 no.3:210 '63.

1. Institute of Physics and Astronomy of the Estonian Academy of Science, U.S.S.R.

KRISTOFEL', N.N.; REBANE, K.K.

Some problems of the theory of luminescence centers in crystalline phosphors. Cs cas fys 13 no.3:241-256 '63.

1. Institut fiziki i astronomii, Akademiya nauk ESSR, Tartu.

KRISTOFEL', N.N.; REBANE, K.K.; SIL'D, O.I.; KHIZHNYAKOV, V.V.

Causes of the difference between the half-width of the absorption and emission bands of crystal phosphors. Opt. i spektr. 15 no.4:569-572 O '63. (MIRA 16:11)

PETRASHEN', M.I., KRISTOFEL', N.N.; ABARENKOV, I.V.

Hartree-Fock's equations for nonmetal crystals. Vest. LGU 18 no.10:5-15 '63. (MIRA 16:8)

(Crystallography)

KRISTOFEL', N.N.

Calculating the lattice distortion around an impurity in an ionic crystal. Fiz. tver. tela 5 no.8:2367-2369 Ag '63. (MIRA 16:9)

1. Institut fiziki i astronomii AN Estonskoy SSR, Tartu.
(Ionic crystals--Defects)

ACCESSION NO: AT3013077 S/2613/62/000/021/0003/0011

AUTHOR: Kristofel', N. N.

TITLE: More precise formulation of an excited state luminescence center theory

SOURCE: AN EstSSR. Institut fiziki i astronomii. Trudy*, no. 21, 1962, 3-11

TOPIC TAGS: luminescence center, activator, adiabatic potential, degeneration, equilibrium configuration, anisotropy, admixture electron cloud

ABSTRACT: Formulas have been presented for the parameters determining the adiabatic potential of luminescence centers in F_{1u}-state with cubical symmetry (NaCl lattice type), taking into account the asymmetry of the interaction between the activator and its proximity. The expression for the luminescence center adiabatic potential is reproduced from the author's previous work (Trudy* IFA AN ESSR, No. 10, 3, 1959; No. 11, 180, 1960). The possibility for minimizing the adiabatic potential on various linear combinations of p-function degenerate states is investigated. A solution is presented first for a single oscillator model and subsequently for non-fully symmetric oscillations contributing to the shift in ion equilibrium configuration. An equilibrium configuration for the ions in the F_{1u}-state is derived,

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ACCESSION NO: AT3013077

indicating the Jan-Teller effect to be completely due to the anisotropy of the admixture electron clouds. Orig. art. has: 18 formulas.

ASSOCIATION: AN EstSSR. Institut fiziki i astronomii (AN EstSSR. Institute of Physics and Astronomy)

SUBMITTED: 01Mar62 DATE ACQ: 11Sep63 ENCL: 00

SUB CODE: PH NO REF SOV: 006 OTHER: 000

Card 2/2

ACCESSION NO: AT3013078 S/2613/62/000/021/0012/0019

AUTHOR: Kristofel', N. N.

TITLE: Selection rules for nonadiabatic transitions

SOURCE: AN EstSSR. Institut fiziki i astronomii, Trudy*, no. 21, 1962, 12-19

TOPIC TAGS: nonadiabatic transition, point group, electronic state, optical transition

ABSTRACT: The problem of nuclear vibration symmetry permitting nonadiabatic transitions from α to β electronic states has been considered. The investigation was conducted in conformity with admixture centers with small radii in ionic crystals, and utilized the rule of electron-vibration transition selection of forbidden rigid lattices. The electron wave function is expanded in power series, in terms of normal coordinates of vibrating nuclei. These are then transformed through a symmetric operation to an irreducible point group symmetry representation of admixture center-quasimolecules. Thus it is shown that in the approximate Condon, nonadiabatic transitions between electronic states α and β, whose symmetry coincides with the perturbation symmetry, can be resolved to a corresponding optical transition

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$$\boxed{\Gamma_1 \times \Gamma_2 \times \Gamma_2} \qquad (1).$$

Examples are cited for the resolution of such transitions in alkali-halide normal luminescence centers. "The author expresses his gratitude to K. K. Rebane for his influence on this work." Orig. art. has: 10 formulas.

ASSOCIATION: AN EstSSR. Institut fiziki i astronomii (AN EstSSR. Institute of Physics and Astronomy)

SUBMITTED: 29Apr62	DATE ACQ: 11Sep63	ENCL: 00
SUB CODE: PH	NO REF SOV: 009	OTHER: 006

Card 2/2

ACCESSION NR: AT4020791 S/2613/63/000/023/0003/0017

AUTHOR: Zavt, G. S.; Kristofel', N. N.

TITLE: Localized vibrations in ionic crystals with an isotopic defect

SOURCE: AN EstSSR. Institut fiziki i astronomii. Trudy*, no. 23, 1963. Issledovaniya po lyuminestsentsii (Research in luminescence), 3-17

TOPIC TAGS: crystal, ionic crystal, crystal vibration, crystal defect, crystal structure isotopic defect, alkali halide crystal lattice

ABSTRACT: The authors develop a theory for the localized modes of vibration which arise in NaCl type ionic crystals in the case of an isotopic substitution of one of the lattice ions. Use of the Green function in harmonic approximation was proposed by Lifshits (I. M. Lifshits, ZHETF, 17, 1017; 1076, 1947; ZHETF, 18, 243, 1948). Before proceeding to an analysis of the vibrations in defective crystals, the authors reduce somewhat the equations of motion of an ideal lattice. It is shown that, for the development of localized vibrations in lattices with similar ion masses, the impurity must be, on the average, twice as light as the substituted ion. There is a detailed study of the localized mode frequency as a function of the impurity mass for NaF. Computations are made for the localized vibration mode frequencies of U-centers of H^- and D^- types for 10 ionic lattices,

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ACCESSION NR: AT4020791

and it is shown that the results of these calculations are in agreement with available experimental data; with the exception of KI the difference nowhere exceeds 10%. The authors also note that a triplet, and not a single frequency, is observed in the spectra. The authors attribute this splitting to a change in the interaction constants around the defect. "The authors wish to express their gratitude to M. I. Kornfel'd and D. N. Mirlin for their discussion of the problems raised in the article." Orig. art. has: 2 tables, 1 figure and 28 formulas.

ASSOCIATION: INSTITUT FIZIKI I ASTRONOMII AN ESTSSR (Institute of Physics and Astronomy)

SUBMITTED: 04Jan63 DATE ACQ: 07Apr64 ENCL: 00

SUB CODE: PH NO REF SOV: 002 OTHER: 017

Card 2/2

S/0023/64/000/002/0087/0109

ACCESSION NR: AP4043031

AUTHORS: Rebane, K. K.; Kristofel', N. N.; Trifonov, Ye. D.; Khizhnyakov, V. V.

TITLE: Dynamics of a lattice with impurities and quasi-line electron-vibration spectra of crystals

SOURCE: AN EstSSR. Izv. Seriya fiziko-matematicheskikh i tekhnicheskikh nauk, no. 2, 1964, 87-109

TOPIC TAGS: crystal lattice vibration, impurity spectrum, electron spectrum, line spectrum, crystal lattice theory, Mossbauer effect, Raman scattering

ABSTRACT: This survey article brings up to date an earlier report (N. N. Kristofel' and K. K. Rebane, Fizika shchelochno-galoidny*kh kristallov [Physics of Alkali-Halide Crystals] Riga, 1962, p. 32) in light of three major developments that have occurred during the

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ACCESSION NR: AP4043031

elapsed time. The first is the progress in the theory of crystal-lattice dynamics, particularly the character of distortion of the crystal lattice near impurities, which has made it possible to predict various types of oscillations in electron-vibration and related processes. The second is the application of the Mossbauer effect to the study of local lattice dynamics. The third is the better understanding of the closed connection between the interaction with electron-transition vibrations and the analogous problem of gamma transitions in an atomic nucleus contained in the crystal (optical analog of the Mossbauer line and the Shpol'skiy effect). In addition, the number of experimental researches on the direct study of dynamics of the lattice near crystal defects, including local oscillations, has greatly increased during the past few years. It is pointed out in the conclusions that principal interest attaches to further development of the theory of the purely electronic line and performance of exact experiments aimed at ascertaining how narrow they can be and how close the analogy between the Mossbauer line

Card 2/3

ACCESSION NR: AP4043031

and the purely electronic line actually is. Further development of the theory of vibrations of impurity molecules in crystals and further research with the aid of the Mossbauer effect are urged. The section headings are: 1. Introduction. 2. Local and pseudolocal oscillations. 3. Electron-vibration transitions and local lattice dynamics. 4. Raman scattering of light. 5. Infrared absorption spectra. 6. Mossbauer effect and a few other phenomena. 7. Concluding remarks. Orig. art. has: 2 figures, 2 formulas, and 1 table.

ASSOCIATION: None

SUBMITTED: 12Mar64 ENCL: 00

SUB CODE: OP, SS NR REF SOV: 066 OTHER: 068

Card 3/3

ACCESSION NR: AP4028466 S/0181/64/006/004/1246/1248

AUTHORS: Kristofel', N. N.; Tyurkson, E. E.

TITLE: Computation of the properties of the pair vacancy in alkali halide crystal

SOURCE: Fizika tverdogo tela, v. 6, no. 4, 1964, 1246-1248

TOPIC TAGS: alkali halide crystal, crystal defect, pair vacancy, equilibrium point shift, ionic vibrational frequency, KCl crystal, induced dipole, ion dipole interaction

ABSTRACT: The properties of the pair vacancy, a structural defect of adjacent anion and cation commonly occurring in alkali-halide crystals, are investigated. The pair vacancy and its nearest neighbors are shown in Fig. 1. of the Enclosure. At sufficiently close neighboring ions, the electric field due to each of the two vacancies is non-zero. Thus, an ion-dipole interaction occurs between the charges of the defect and the induced dipoles. The interaction energy is given by

$$W_d = -\frac{e^2}{2}\sum_i \beta_i \left(\frac{\mathbf{R}_i}{R_i^3} - \frac{\mathbf{R}'_i}{R_i'^3}\right)^2,$$

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ACCESSION NR: AP4028466

where β_s is the polarizability of the s-th ion, and R_s and R'_s are the distances from the centers of the vacancies to the s-th ion. Sufficient accuracy is obtained by considering only the 10 nearest neighbors and their remaining 34 nearest neighbors. The shift of the equilibrium position from that of the ideal crystal is shown in the figure for each of the 4 non-equivalent groups: 1; 2, 3, 4, 5; 6, 7, 8, 9; 10. An expression for this shift is given assuming the shift is directed along the coordinate axes as indicated in the figure, i. e., the attraction between ions of groups 2 and 6 is ignored. An equation for the vibrational frequency of the ions is also given. The form of the energy for pair vacancy formation is indicated, and numerical calculations are made for the KCl crystal. The authors are grateful to A. I. Stekhanov for discussions leading to the formulation of the computations. Orig. art. has: 25 equations and 1 diagram.

ASSOCIATION: Institut fiziki i astronomii AN ESSR, Tartu (Institute of Physics and Astronomy AN ESSR)

SUBMITTED: 28Nov63 DATE ACQ: 27Apr64 ENCL: 01

SUB CODE: GP NO REF SOV: 006 OTHER: 010

Card 2/3

ACCESSION NR: AP4028466 **ENCLOSURE:** 01

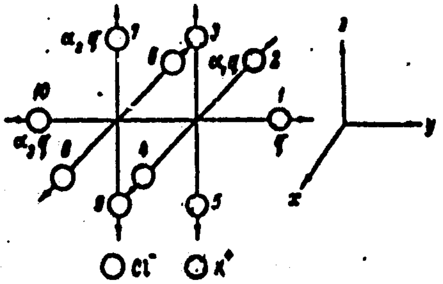

Fig. 1 : The pair vacancy and its closest neighbors in the KCl crystal.

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ACCESSION NR: AP4020926 S/0051/64/016/002/0256/0259

AUTHOR: Kristofel', N.N.; Zavt, G.S.

TITLE: Concerning interpretation of vibronic transitions in impurities on the basis of the dynamic theory of nonideal lattices

SOURCE: Optika i spektroskopiya, v.16, no.2, 1964, 256-259

TOPIC TAGS: vibronic transitions, phonon spectrum, lattice vibration, impurity center, lattice defect, nonideal lattice, imperfect crystal, quasiline spectra, edge emission, edge luminescence

ABSTRACT: The phonon spectrum of a crystal with a number of defects may differ substantially from the spectrum of an ideal crystal by the presence of a number of "local" frequencies. Hence in considering the vibronic transitions in impurity centers, for example, one must take into consideration the vibrations of a nonideal crystal. In the present paper there is considered the distortion of the crystal lattice vibrations in the vicinity of defects (impurity centers). It is shown that the displacements of the host atoms close to the defect as a function of frequency may have a number of sharp maxima. The frequencies corresponding to these maxima either de-

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ACCESSION NR: AP4020926

termine the effective frequencies of the impurity center or are evinced in form of narrow quasilines (in the respective cases of centers with large and small Stokes losses). Some experimental and theoretical data for different types of luminescence centers (mercury-like, F and rare earth centers) are discussed and analyzed from the standpoint of the considerations adduced. It is suggested that the frequencies evinced in the vibrational structure of the edge emission spectra of some non-activated crystals (ZnS, CdS, ZnO) may be associated with the above mentioned maxima. "The authors are grateful to K.K.Rebane for detailed discussion of some of the problems involved and to Ch.B.Lushchik for valuable suggestions." Orig.art.has: 2 formulas and 1 table.

ASSOCIATION: none

SUBMITTED: 14Jun63 DATE ACQ: 02Apr64 ENCL: 00

SUB CODE: PH NR REF SOV: 010 OTHER: 012

Card 2/2

ACCESSION NR: AT4004329 S/2613/63/000/020/0122/0131

AUTHOR: Kristofel', N. N.

TITLE: Theory of electron-oscillatory bands forbidden in a static lattice

SOURCE: AN EstSSR. Institut fiziki i astronomii. Trudy*, no. 20, 1963. Issledovaniya po teoreticheskoy fizike, 122-131

TOPIC TAGS: electron band, phosphor, forbidden transition, impurity center, crystal lattice, lattice dynamics, electron oscillatory transition, static lattice, Jahn Teller effect

ABSTRACT: In this article, two topics are considered: first, the symmetry of vibrations caused by the breakdown of the Condon approximation and leading to electron-oscillatory transitions forbidden in the static lattice between the levels of small impurity centers; second, the connection between the Jahn-Teller effect and the breakdown of the Condon approximation. The electron-oscillatory bands associated with the transitions forbidden in the static lattice are generated in activating impurities in fluorescent crystals. The intensity of these bands increases with temperature, because the vibrations of the nuclei turn the forbidden bands into permitted ones. As a result of these vibrations, the electron wave functions are deformed and the electron matrix element of transition becomes dependent on the coordinates of the nuclei. In other words, the Condon approximation breaksdown. The

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ACCESSION NR: AT4004329

symmetry of vibrations is investigated to determine what kind of symmetries can remove the prohibition from a certain transition. The analysis is carried out by means of the theory of groups. In the static crystal lattice and dipole approximation, transitions between states of the same evenness are forbidden (if the group of the symmetry of the center contains the operation of inversion). This prohibition is removed by odd vibrations. However, if the transition is forbidden by other selection rules besides evenness, then only even vibrations can remove the prohibition. The motions of only those ions included in the region of the impurity electron cloud are essential for the deviation from the Condon approximation. To determine the symmetry of the vibrations and their number, the impurity center is considered as a quasi-molecule. The Jahn-Teller effect consists in lowering the equivalent symmetry of the center and splintering the adiabatic potential. According to the Condon approximation, the splintering does not take place in the absorption spectrum. If the Condon approximation is disturbed by the same incompletely symmetrical vibrations which lead to the Jahn-Teller effect, the absorption band consists of the half-bands. In the opinion of the author, the Jahn-Teller effect, the breakdown of the Condon approximation, and the deviation from the adiabatic state should be considered as mutually connected phenomena. "The author thanks K. K. Rebane and Ch. B. Lushchik for considering these questions." Orig. art. has: 12 formulas.

Card 2/3

ACCESSION NR: AT4004329

ASSOCIATION: Institut fiziki i astronomii AN EstSSR (Institute of Physics and Astronomy AN EstSSR)

SUBMITTED: 10 Mar62 DATE ACQ: 14Jan64 ENCL: 00

SUB CODE: GP NO REF SOV: 006 OTHER: 001

Card 3/3

[illegible] and oscillations from the entire phonon spectrum may par-

[illegible]

Ga^+ in the $^1S_0$ state in a KCl lattice site. The analysis is limited the calculation of the properties, and especially the distortion [illegible]

REBANE, K.K.; KRISTOFEL', N.N. [Kristoffel, N.]; TRIFONOV, Ye.D.;
KHIZHNYAKOV, V.V.

Dynamics of a lattice with impurities and the quasi-line electron-vibration spectra of crystals. Izv. AN Est. SSR. Ser. fiz.-mat. i tekh. nauk 13 no.2:87-109 '64.
(MIRA 17:9)

1. Corresponding Member of the Academy of Sciences of the Estonian S.S.R. (for Rebane).

L 6321-66 EPA(s)-2/EWT(m)/EWP(t)/EWP(b) IJP(c) JD/JG
ACCESSION NR: AP5019863 UR/0181/65/007/008/2444/2449

56
54

AUTHOR: Zavt, G. S.; Kristofel', N. N.; Khizhnyakov, V. V.

TITLE: Contribution to the theory of the width of infrared U-center absorption bands B

SOURCE: Fizika tverdogo tela, v. 7, no. 8, 1965, 2444-2449

27

TOPIC TAGS: potassium chloride, potassium bromide, activated crystal, line width, IR spectrum, absorption line, crystal defect, impurity center, crystal vibration, phonon interaction

ABSTRACT: The purpose of the article was to explain why recent experimental measurements of the line width in systems KCl-H, D and KBr-H, D (D. N. Mirlin and I. I. Reshina, FTT v. 5, 3352, 1963; v. 6, 945 and 3078, 1964) have led to results that did not agree with previous theoretical explanations, namely that the width of the infrared bands of U-center absorption increases more rapidly with temperature than follows from any acceptable decay scheme. The authors therefore conclude that the dominating contribution to the line width, at least at high temperatures, is made by processes of higher orders, namely 4-phonon processes for D centers and 5-phonon processes for H-centers. They prove this point of view by analyzing a formula for the line width, which they derive in the following approximations: It

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L 6321-66
ACCESSION NR: AP5019863

2

is assumed that the defect differs from the substituted ion in mass only. Inasmuch as the impurity level is well localized, it is assumed that the defect participates only in the local vibrations, and the crystalline vibrations at atoms neighboring on the defect are not perturbed. This means that in the case of D-centers it is necessary to take into account processes in which two and three phonons are produced, and in the case of H-centers--three and four phonons. The anharmonic interactions of 3rd, 4th, and 5th orders are analyzed in the usual manner using the two-time Green's functions. The theoretical curve revised in this manner is in good agreement with the experimental data. "The authors thank D. N. Mirlin for useful discussions." Orig. art. has: 1 figure, 9 formulas, and 1 table.

ASSOCIATION: Institut fiziki i astronomii AN ESSR, Tartu (Institute of Physics and Astronomy AN ESSR)

SUBMITTED: 14Jan65	ENCL: 00	SUB CODE: SS, OP
NR REF SOV: 007	OTHER: 013	

BVK
Card 2/2

L 6332-66 EWT(m)/EWP(t)/EWP(b) IJP(c) JD/JG
ACCESSION NR: AP5019874

UR/0181/65/007/008/2519/2522

44,55

AUTHOR: Kristofel', N. N.

TITLE: Vibration symmetry and Raman scattering spectra of alkali-halide crystals with impurities

SOURCE: Fizika tverdogo tela, v. 7, no. 8, 1965, 2519-2522

21,44,55

TOPIC TAGS: Raman spectrum, alkali halide, crystal impurity, crystal symmetry, phonon, Brillouin zone, spectral line

ABSTRACT: The author investigates Raman scattering in alkali-halide crystals of the NaCl type with a substitutional impurity at the lattice point. It is assumed that the types of point symmetry of the crystalline (pseudolocal) and local vibrations are the same as in a quasi-molecule made up of the impurity and its neighbors, with which it interacts. Using the table constructed by R. Loudon (Proc. Phys. Soc. v. 84, 379, 1964) and the compatibility tables of Bouckaert et al. (Phys. Rev. v. 50, 58, 1936) the author determines the phonon symmetries at the different points of the Brillouin zone and presents the selection rules for the quasi-linear spectrum of Raman scattering of these crystals. It is shown that the phonons at the points k = 0 and X made no contribution to odd-order lines, making it possible to

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L 6332-66

ACCESSION NR: AP5019874

12

explain some experimentally observed rules for pseudolocal oscillations, previously observed by the author (Tr. IFA AN ESSR No. 18, 149, 1962). "The author is grateful to A. I. Stekhanov 44,2 for a discussion of the problem and to K. K. Rebane and G. S. Zavt for a discussion of the work." Orig. art. has: 2 tables. 44,55 44,55

ASSOCIATION: Institut fiziki i astronomii AN ESSR, Tartu (Institute of Physics and Astronomy AN ESSR) 44,55

SUBMITTED: 27Jan65 ENCL: 00 SUB CODE: OP, SS

NR REF SOV: 015 OTHER: 005

nw

Card 2/2

KRISTOFEL', N. [Kristoffel,N.]; GODKAINS, A.

Theory of complex luminiscence centers. Part 1. Izv. AN Est. SSR. Ser. fiz.-mat. i tekh. nauk 14 no. 4:507-525 '65
(MIRA 19:2)

1. Institut fiziki i astronomii AN Estonskoy SSR. Submitted November 23, 1964.

Card 1/2

[illegible] of the $P_1 \to S_0$ band of [illegible]. The results are found to agree with experiment at low temperatures. The author

L 23527-66 EWT(1)

ACC NR: AT6008334 SOURCE CODE: UR/2613/64/000/027/0085/0098

63
60
B+1

AUTHOR: Kristofel', N. N.

ORG: none

TITLE: Possibility of the Jahn-Teller effect for the band states of crystals

SOURCE: AN EstSSR. Institut fiziki i astronomii. Trudy, no. 27, 1964. Issledovaniya po teorii tverdogo tela (Research on the theory of solids), 85-98

TOPIC TAGS: phonon spectrum, energy band structure, crystal theory, crystal lattice vibration, crystal, crystal symmetry, band spectrum, electron interaction, phonon interaction

ABSTRACT: The author considers the possibility for a reduction in the symmetry of the nuclear arrangement and a corresponding splitting of the electron levels as a result of interaction between the degenerate electron state of a perfect crystal and nonholosymmetric lattice vibrations. The differences between wide and narrow bands are considered. In the case of wide bands, electron-phonon interaction is considered as a perturbation for the band states. Only optical threshold vibrations may take part in the Jahn-Teller effect. The effect is infinitely small for a single electron, but may be finite for a sufficiently large number of electrons in a degenerate band. In the case of narrow bands, electron-phonon interaction is first considered in a single cell and then interaction between different cells is analyzed. Vibrations of the appropriate symmetry from the entire phonon spectrum may contribute to the effect. The quasi-

2

Card 1/2

L 23527-66

ACC NR: AT6008834

3

molecular model which was developed earlier for impurity centers is applicable here (polarons and excitons of small radius, "intramolecular" states, etc.). Some experiments for detection of the effect are discussed. The author is grateful to K. K. Rebane as well as to participants in seminars at the Department of Quantum Mechanics, Leningrad State University and the Institute of Physics and Mathematics AN MSSR for discussion of the work. Orig. art. has: 8 formulas.

SUB CODE: 20/ SUBM DATE: 13Nov63/ ORIG REF: 009/ OTH REF: 007

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L 23526-66 EWT(1)/EWT(m)/T/EWP(t) IJP(c) GO/JD

ACC NR: AT6008335 SOURCE CODE: UR/2613/64/000/027/0099/0107

49

48

B+1

AUTHOR: Kristofel', N. N.; Tyurkson, E. E.

ORG: none

TITLE: Calculation of vibration frequency and lattice distortions near a vacancy pair in potassium chloride ,1

27

SOURCE: AN EstSSR. Institut fiziki i astronomii, Trudy, no. 27, 1964. Issledovaniya po teorii tverdogo tela (Research on the theory of solids), 99-107

TOPIC TAGS: crystal lattice vibration, crystal lattice distortion, crystal lattice vacancy, potassium chloride, vibration frequency, approximation method

21, 44, 55

ABSTRACT: The authors use the quasimolecular approximation method, developed originally for impurity centers, to calculate lattice distortions and vibration frequency for ions near a vacancy pair in a sodium chloride type crystal. Only displacements of the closest neighbors around the vacancy pair are considered (there are 10 nearest ions) and the remaining ions are assumed to be fastened in equilibrium positions corresponding to an ideal crystal. The calculations are based on a cation-anion vacancy pair in KCl. It is found that the distortion of the lattice near the defect gives a symmetry of C_{4v}. The frequency of the actual vibrations near the defect is $2.03 \cdot 10^{13}$ $\sec^{-1}$. The coupling energy of the vacancy pair is found to be 8.73 ev. The

2

Card 1/2

L 23526-66

ACC NR: AT6008335

authors are grateful to A. I. Stekhanov who prompted the undertaking of this calculation. Orig. art. has: 2 figures, 11 formulas.

SUB CODE: 20/ SUBM DATE: 14Nov63/ ORIG REF: 007/ OTH REF: 010

Card 2/2

L 32949-66 EWT(l) IJP(c)

ACC NR: AP6014856 SOURCE CODE: UR/0023/65/000/004/0507/0527

26

B

AUTHOR: Kristofel', N. -- Kristoffel, N.; Godkalns, A.

ORG: Institute of Physics and Astronomy, Academy of Sciences Estonian SSR (Institut fiziki i astronomii Akademii nauk Estonskoy SSR)

TITLE: On the theory of complex luminescence centers 21 Part I

SOURCE: AN EstSSR. Izvestiya. Seriya fiziko-matematicheskikh i tekhnicheskikh nauk, no. 4, 1965, 507-527

TOPIC TAGS: luminescence center, impurity center, perturbation theory, crystal lattice vacancy

ABSTRACT: The paper discusses an impurity center in a static NaCl-type lattice, consisting of a divalent activator ion at a lattice point and a vacancy of a like ion of the lattice. General formulas are derived for the energy of a center with a mercury-like activator in the ground and split excited electron states. The corresponding transition energies for centers with C_{4v} and C_{2v} symmetry are derived in terms of the wave functions of the ions and considering the effect of the field of the point lattice. The energy of a central ion in a lattice with defects, the energy of an impurity ion with an associated vacancy (considering the ground and excited state of the impurity),

Card 1/2

L 32949-66

ACC NR: AP6014856

0

and the energy of optical absorption were calculated. Orig. art. has: 91 formulas.

SUB CODE: 20/ SUBM DATE: 23Nov64/ ORIG REF: 032/ OTH REF: 010

Card 2/2

L 04146-67 EWT(m)/T/EWP(t)/ETI IJP(c) JD

ACC NR: AP6026670 SOURCE CODE: UR/0181/66/008/008/2271/2279

62
61.
B

AUTHOR: Zavt, G. S.; Kristofel', N. N.

ORG: Institute of Physics and Astronomy, AN ESSR, Tartu (Institut fiziki i astronomii AN ESSR)

v1 v1

TITLE: Distortion of band vibrations of NaCl-type crystals by monovalent impurities

SOURCE: Fizika tverdogo tela, v. 8, no. 8, 1966, 2271-2279

TOPIC TAGS: sodium chloride, single crystal lattice, impurity band, crystal impurity, crystal lattice defect, Green function, CRYSTAL LATTICE VIBRATION

ABSTRACT: An analysis is given of the distortion of band vibrations of NaCl-type crystals by monovalent impurities in the lattice points. It is based on a previous study by Zavt (FTT, 7, 2109, 1965.) in which it was shown that, in addition to exciting local vibrations, the impurities act to modify lattice vibrations in the region of lattice defects. On this basis, the distortion of vibrations by defects is studied by calculating the spectral density of the atom displacements in the region of lattice defects (or the eigenvectors of the dynamic matrix). The method employed to determine these eigenvectors is based on the introduction of modified Green functions. A distinctive feature of the method is that the eigenvectors (or their combinations) consitute the

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ACC NR: AP6026670

particular solution of the equations of motion. Graphs showing the modified Green functions for KCl are presented, together with graphs that show the nature of the calculated band vibrations of various types of symmetry. The authors are indebted to E. E. Saareste for programming the calculations of the Green's functions. Orig. art. has: 3 figures and 26 formulas.

SUB CODE: 20/ SUBM DATE: 16Oct65/ ORIG REF: 013/ OTH REF: 010

Card 2/2

ACC NR: AP7004995 SOURCE CODE: UR/0048/66/030/009/1533/1536

AUTHOR: Kristofel', N.N.

ORG: none

TITLE: Local levels of activator neighbors in alkali phosphors /Report, Fourteenth All-Union Conference on Luminescence (Crystal Phosphors) held at Riga, 16-23 Sept.1965/

SOURCE: AN SSSR. Izvestiya. Seriya fizicheskaya, v. 30, no.9, 1966, 1533-1536

TOPIC TAGS: luminescent crystal, potassium chloride, thallium, absorption band, electron energy level, mathematic physics

ABSTRACT: The author has calculated the energies of the 3p states of the Cl^- ions that are nearest neighbors to Tl^+ impurity ions in a KCl lattice. The calculations have been described in more detail elsewhere (N.N.Kristofel', Tr. In-ta fiz. i astron. AH EstSSR, No.32 (1966)). The calculations are of interest because a knowledge of induced local levels is necessary for an understanding of the release of excitation from impurities and the trapping of holes, and for the interpretation of spectral bands associated with energy transport (trapped excitons). For the calculations, the Hartree-Fock determinant was formed with one-electron wave functions centered on separate ions and calculated with the effect of the field of the point lattice taken into account, and the off-diagonal energy matrix elements were neglected. In this approximation the valence band reduces to a level, and the approximation is therefore

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ACC NR: AP7004995

suitable only when the valence band is narrow. The numerical results are accordingly regarded as merely indicative. The calculations indicated that the valence band lies 10.6 eV below the vacuum level; this is in good agreement with the position of the top of the valence band as calculated by L.Howland (Phys. Rev., 109, 1927 (1958)). The calculated positions of the 3s levels are 0.72 eV above the valence band and 0.71 eV below it. After some discussion it is concluded that on the present model the "transfer" D absorption band of KCl:Tl must be ascribed to an electronic transition from an induced local level of a Cl^- ion neighboring a Tl^+ ion. It is suggested that induced local levels may affect the x-ray spectrum and that relevant information might also be obtained from paramagnetic resonance studies. The author thanks K.K.Rebane, N.Ye.Lushchik and Ch.B.Lushchik for discussions. Orig. art. has: 4 formulas.

SUB CODE: 20 SUBM DATE: none ORIG. REF: 013 OTH REF: 007

Card 2/2

ACCESSION NR: AT4020807 S/2613/63/000/023/0216/0218

AUTHOR: Kristofel', N. N.; Tyurkson, E. E.

TITLE: Calculation of the wave functions of ions in the calcium fluoride crystal

SOURCE: AN EstSSR. Institut fiziki i astronomii. Trudy*, no. 23, 1963. Issledovaniya po lyuminestsentsii (Research in luminescence), 216-218

TOPIC TAGS: wave function, ion wave function, calcium fluoride, fluorite, fluorite ion wave function, calcium fluoride crystal lattice

ABSTRACT: In connection with the use of activated fluorite crystals in quantum generators, there has been an increased interest in recent times in the study of the various properties of CaF_2. Fluorite is one of the ionic crystals. In calculating its different characteristics in a zero approximation, it is possible to call upon the wave functions of the ions Ca^{++} and F^-, with proper consideration of the Madelung field of the surrounding ionic lattice. As the result of a standard calculation, the details of which are not discussed in the article, the authors obtained the data for normalized radial functions (with allowance for the field of the crystal) shown in Table 1 of the Enclosure. As in the case of alkali halide crystals, as compared with the free ions, the anion in the crystal is "compressed" and the cation is "extended". Some notion of the quality of the wave functions obtained

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ACCESSION NR: AT4020807

(for internal shells the corresponding functions of the free ions are used) may be derived from a calculation of the diamagnetic susceptibility of the CaF_2 crystal. The diamagnetic susceptibility of the ion was calculated according to the formula:

$$\underline{\chi = -\frac{e^2 a_0^2}{6 \mu c^2} L \int^{\infty} U(r) r^2 dr,}$$

where где $\underline{U(r) = \sum_{nl} 2(2l+1) P^2_{nl}(r),}$

and for CaF_2 $\underline{\chi = \chi(Ca^{++}) + 2\chi(F^-)}.$

The results are given in Table 2 of the Enclosure ($-\chi \cdot 10^{-6}$ cm^{-3} mole). Orig. art. has: 2 tables and 3 formulas.

ASSOCIATION: Institut fiziki i astronomii AN EstSSR (Institute of Physics and Astronomy, AN EstSSR)

SUBMITTED: 08Jun63 DATE ACQ: 07Apr64 ENCL: 02

SUB CODE: PH NO REF SOV: 003 OTHER: 003

Card 2/4

ACCESSION NR: AP4020807 **ENCLOSURE: 01**

TABLE 1

Ion F$^-$ ион F$^-$:

$0<r<1{,}0 \quad f_{2p}(r)=1{,}114\,f^{0}_{2p}(r),$

$1{,}0<r<5{,}0 \quad f_{2p}(r)=2{,}301\exp(-1{,}126r+1{,}166r^{-1}-1{,}030r^{-2}),$

$r>5{,}0 \quad f_{2p}(r)=2{,}368\left(1+\frac{1}{1{,}126r}\right)\exp(-1{,}126r),$

$0<r<1{,}2 \quad f_{2s}(r)=1{,}020\,f^{0}_{2s}(r),$

$1{,}2<r<4{,}0 \quad f_{2s}(r)=-8{,}074\exp(-1{,}632r+0{,}574r^{-1}-1{,}149r^{-2}),$

$r>4{,}0 \quad f_{2s}(r)=-8{,}676\exp(-1{,}632r);$

Ion Ca^{++} Ион Ca^{++}:

$0<r<1{,}2 \quad f_{3p}(r)=0{,}896\,f^{0}_{3p}(r),$

$1{,}2<r<3{,}4 \quad f_{3p}(r)=-3{,}735r^{1{,}860}\exp(-1{,}621r+$
$+0{,}205r^{-1}-0{,}094r^{-2}),$

$r>3{,}4 \quad f_{3p}(r)=-3{,}768r^{1{,}860}(1+0{,}131r^{-1}+$
$+0{,}043r^{-2}+0{,}005r^{-3})\exp(-1{,}621r).$

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ACCESSION NR: AT4020807 ENCLOSURE: 02

TABLE 2

	calculated by using f"nl	calculated by using f"nl	experimentally (F. Zeyts, Sovremennaya teoriya tverdogo tela, GITTL, 1949)
$\chi(F^-)$ $\chi(Ca^{++})$	17,0 12,1	7,96 15,4	—
$\chi(CaF_2)$	46,1	31,8	24,4

Card 4/4

ACCESSION NR: AP3002667 S/0054/63/000/002/0005/0015

AUTHORS: Petrashen', M. I.; Kristofel', N. N.; Abarenkov, I. V.

TITLE: The Hartree Fock equations for nonmetallic crystals

SOURCE: Leningrad. Universitet. Vestnik. Seriya fiziki i khimii, no. 2, 1963, 5-15

TOPIC TAGS: Hartree Fock equation, nonmetallic crystal, electron zone theory, electron state, wave function

ABSTRACT: In studying crystals as many-electron systems, there has been some tendency to use other methods than the Hartree-Fock one-electron approximation as being more reliable. The authors have analyzed the Hartree-Fock scheme for a crystal, and they have obtained a one-electron zone theory as an approximation to the Hartree-Fock theory. The approach is similar to the Hund-Milliken approximation for a molecule. The authors have based their work on the results of C. Roothan (Rev. mod. phys., 23, 69; 1951; and 32, 179, 1960). They have shown that the information given by the one-electron zone theory derives from a direct examination of the Hartree-Fock equations and that different crystal states (including

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ACCESSION NR: AP3002887

the excited state) may be obtained from the scheme. In examining the Hartree-Fock equations, the authors investigated the energy spectrum of a crystal on the basis of a model of noninteracting electrons in a periodic field. The authors thus conclude that all results of the one-electron zone theory concerning the structure of spectra of a crystal can be obtained from examination of the system of Hartree-Fock equations if it is written in proper form, accounting for symmetry. Orig. art. has: 21 formulas.

ASSOCIATION: Leningradskiy gosudarstvennyy universitet (Leningrad State University)

SUBMITTED: 01Dec62 DATE ACQ: 24Jul63 ENCL: 00

SUB CODE: PH NO REF SOV: 002 OTHER: 005

Card 2/2

KRISTOFFEL, N.

Sixth All-Union Conference on Semiconductor Theory.
Izv. AN Est. SSR. Ser.fiz.-mat.i tekh.nauk 14
no.2:312-314 '65. (MIRA 19:1)

CZECHOSLOVAKIA

SMOLKOVA, E; KRISTOFIKOVA, L; FELTL, L; GRUBNER, O

1. Institute of Physical Chemistry, Czechoslovak Academy of Sciences, Prague (for Grubner); 2. Institute of Analytical Chemistry, Charles University, Prague (for others)

Prague, Collection of Czechoslovak Chemical Communications, No 2, February 1966, pp 450-456

"Determination of the surface of powdery substances by the method of thermal desorption, using organic vapors as the sorbates."

[illegible] [illegible]

Department of Physics, Chair of Marine and Inland Water Physics, 55

28.1000

22926
S/123/61/000/007/017/026
A004/A104

AUTHORS: Kazakevich, V.V., Kornilov, R.V., Kristoforov, N.G.

TITLE: Electronic extremum regulator

PERIODICAL: Referativnyy zhurnal, Mashinostroyeniye, no. 7, 1961, 5, abstract 7D48 (V sb. "Teoriya i primeneniye diskretn. avtomat. sistem," Moscow, AN SSSR, 1960, 558 - 569)

TEXT: The authors describe an electronic extremum regulator whose operation principle is based on the searching of the optimum conditions with extremum storage. The electronic extremum regulator consists of 1) signum relay to determine the sign of the input magnitude increment and the shaping of the signal of motion admissibility or inadmissibility; 2) commutator (including a master oscillator, intermediate stage, relaxation relay with two stable states) intended for the periodical reversing of the system if there are signals corresponding to the motion of the system in one direction; 3) triggering device. The authors present a schematic system of the electronic extremum regulator and state the main parameters. They give an account of the test results of the electronic extremum

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S/123/61/000/007/017/026
A004/A104

Electronic extremum regulator

regulator in the closed control system of an electronic simulating installation. There are 14 figures and 7 references.

G. Buberban

X

[Abstracter's note: Complete translation]

Card 2/2

KRISTOFOVA, Hana; HILGERT, I.

The role of lipoprotein and deoxyribonucleic acid in antigenicity of the Ehrlich ascites tumour. Folia biol. (Praha) 11 no.3:237-239 '65

1. Institute of Experimental Biology and Genetics, Czechoslovak Academy of Sciences, Prague.

RADEJ, Zdenek, inz.; KRISTOFOVA, Zdena, inz.

Fraction of hydroxy acids and lactones in black liquor. Papir a celulosa 19 no. 6:152-153 Je '64.

1. Research Institute of Paper and Cellulose, Bratislava.

L 21158-66 T IJP(c)

ACC NR: AP6010939 SOURCE CODE: CZ/0014/65/000/003/0092/0095

AUTHOR: Kristofovic, Gustav

33
13

ORG: none

TITLE: Electric exposure meter for a positive photographic process

SOURCE: Sdelovaci technika, no. 3, 1965, 92-95

TOPIC TAGS: exposure meter, electronic circuit, photography

ABSTRACT: This paper presents the circuits and an explanation of the principle of an electric exposure meter for objective measurement of the correct exposure of positives and simultaneous determination of correct gradation. Orig. art. has: 10 figures and 2 formulas. [JPRS]

SUB CODE: 14, 09 / SUBM DATE: none / ORIG REF: 009

Card 1/1

KRISTOFOROVIC, I.

Reply to M. Arsenijevic's second review of Ivan Kristoforovic's book *Mlinarstvo (Flour Mills)*. p. 765.
TEHNIKA, Beograd, Vol. 10, no. 5, 1955.

SO: Monthly List of East European Accessions, (EEAL), LC, Vol. 4, no. 10, Oct. 1955, Uncl.

KRISTOFOVIC, O.

A practical design for r-f and i-f circuits in a television receiver. p.144.
(Sdelovaci Techinika, Vol. 5, No. 5, May 1957, Praha, Czechoslovakia)

SO: Monthly List of East European Accessions (EEAL) LC. Vol. 6, No. 9, Sept. 1957. Uncl.

KRISTOFOVIC, Gustav

Transistorized unit for reception of very short waves. Sdel tech 11 no.8:286-291 Ag '63.

KRISTOFFEL, N.

International Symposium on Luminescence. Izv. AN Est. SSR. Ser. fiz.-mat. i tekh. nauk 12 no.2:220 '63. (MIRA 16:10)

KRISTOFFEL, N.

International Conference on the Dynamics of the Crystal Lattice, held at Copenhagen. Izv. AN Est. SSR. Ser. fiz.-mat. i tekh. nauk 12 no.3:352-353 '63. (MIRA 16:11)

GANKINA, N.Z.; DRABKIN, G.M.; KRISTOL, D.I.; LAPINAGOV, P.I.; NEFEDOV, P.K.;
SELUYANOV, M.P.

Standard sections of universal multistory industrial buildings.
Prom. stroi. 40 [i.e. 41], no.5:37-40 My '63. (MIRA 16:5)
(Industrial buildings--Design and construction)

KRISTOL, F.M.

Obtaining purified viscose cellulose. Bum.prom. 29 no.12:
17-20 D '54. (MLRA 8-2)

1. Nachal'nik laboratorii sul'fitno-tsellyuloznogo zavoda
Svetogorskogo tsellyulozno-bumazhnogo kombinata.
(Cellulose)