is applied to the crystal the absorption constants $K_{\parallel}$ and $K_{\perp}$ measured with light polarized parallel and perpendicular to the stress axis are different. This difference $\Delta K = K_{\parallel} - K_{\perp}$ is plotted versus spectral energy for [001] stress in the lower part of Fig. 1. A comparison of $\Delta K(E)$ with the absorption spectrum $K(E)$ in the upper part of Fig. 1 shows that the change of the oscillator strength under applied stress is the dominant effect, whereas a shift of the bands due to a splitting of the excited states is negligible. ΔK is a linear function of the stress. We also note that ΔK differs in sign for the two bands.

Fig. 3 summarizes the temperature dependence of the stress effects. The oscillator strength $f(T)$ for a single band is found from a Gauss-curve analysis using the data of Fußgänger [1]. We find that $\Delta f/f = (f_{\parallel} - f_{\perp})/f$ has the same sign for corresponding bands in NaCl:Cu$^+$ and KCl:Ag$^+$. To explain sign and temperature dependence of $\Delta f/f$ we will discuss three effects: 1. a frequency splitting of the far IR resonance mode, 2. a small off-centre distortion of the defect, and 3. a quadratic electron–lattice interaction. We will show in the discussion of the experimental data that all three effects contribute to the observed dichroism, but the main contribution comes from the first and second effects mentioned above.

3. Theory

To investigate the interaction between the electronic states of the defect and the ionic displacements, it is convenient to classify the electronic wave functions and the normal coordinates $Q(l)$ of the perturbed lattice according to their transformation properties under the elements of the point group of the defect site. For well localized defects it is sufficient to consider the interaction within the octahedral complex Ag$^+$(Cl$^-$)$_6$ or Cu$^+$(Cl$^-$)$_6$ and introduce the symmetry coordinates $q_{\alpha i}$ of the complex which are basis functions of the irreducible representations Γ_α of O$_h$ (i denotes the row index). Small deviations from O$_h$-symmetry due to lattice vibrations and static distortions (Jahn-Teller effect, off-centre displacement) of the lattice cell will be treated as perturbations. The symmetry coordinates $q_{\alpha i}$ are linear combinations of the normal coordinates $Q(l)$ of the perturbed lattice:

$$q_{\alpha i} = \sum_l c_{\alpha i}(l)\, Q(l)\,. \tag{1}$$

Each symmetry coordinate is associated with a distortion with a potential energy $\frac{1}{2}\,\omega_\alpha^2\,q_{\alpha i}^2$ where ω_α is an effective frequency of the complex.

The Hamiltonian H of the system

$$H = H_e + H_l + H_{el} \tag{2}$$

consists of the Hamiltonian of the defect electrons H_e, the lattice Hamiltonian H_l, and the operator of the electron–lattice interaction H_{el}. We expand the electron lattice interaction in the Hamiltonian in terms of the symmetry coordinates $q_{\alpha i}$, taking linear (equation (3a)) and quadratic terms (equation (3b)) into account:

$$H_{el} = H_1 + H_2\,, \tag{3}$$

$$H_1 = \sum_{\alpha,\, i} V_{\alpha i}^-(\mathbf{r})\, q_{\alpha i}^-\,, \tag{3a}$$

$$H_2 = \sum_{\alpha,\, i} \sum_{\beta,\, j} V_{\alpha i\,\beta j}^-(\mathbf{r})\, q_{\alpha i}^-\, q_{\beta j}^+ + \cdots\,. \tag{3b}$$

$\mathbf{r}$ denotes the set of electronic coordinates and the upper sign the parity of the distortion. $V_{\alpha i}^-(\mathbf{r})$ has the same transformation properties as the i-th basis func-

KCl:Ag$^+$

77°K

D   B   A

23°K

77°K

P[001]

100 $\frac{kp}{cm^2}$

150°K

6.0   5.8   5.6   5.4   5.2
◄—— Photon energy (eV)

...sorption constant K and its change ΔK un-
...stress versus photon energy for KCl:Ag$^+$

...l of aggregate centres the sam-
...d for a few minutes at about
...r the melting point and then
...room temperature.

...part of Fig. 1 shows the UV
...NaCl:Cu$^+$ at 77 °K. The main
...eV, called the D-band, corre-
...ansition $\Gamma_1^+ \to \Gamma_5^+$. In the small
...4.5 eV, called the A-band, the
...ons $\Gamma_1^+ \to \Gamma_3^+$ and $\Gamma_1^+ \to \Gamma_5^-$.
...$^+ \to \Gamma_3^+, \Gamma_5^+$, contribute to the
...$^\pm_\alpha$ denotes the transformation
... the unperturbated electronic
...defect under the elements of
...oup O$_h$. When uniaxial stress

...oscillator strength $f_{\parallel} - f_{\perp}$ normalized to
...r strength f plotted versus temperature