tion of $\Gamma_\varkappa^-$, and $V_{\varkappa i \beta j}^-(\boldsymbol{r})$ transforms as the product $q_{\varkappa i}^- \times q_{\beta j}^+$. In this approach no other terms of the same order in the distortions $q_{\varkappa i}$ contribute to our effects.

The zeroth-order electronic wave function $\psi_{\mu i}$ is an eigenfunction of H_e. $\psi_{\mu i}$ describes the electronic state in the static complex and is the i-th basis function of the μ-th irreducible representation. Taking H_{el} as a perturbation and the ionic displacements $q_{\varkappa i}$ as parameters, we obtain a mixing between even and odd electronic states $\psi_{\mu i}$ of the defect:

$$\psi'_{\mu i} = \psi^+_{\mu i} + \sum_{\nu, j} \frac{\langle \psi^-_{\nu j} | H_{el} | \psi^+_{\mu i} \rangle}{E_\mu - E_\nu} \psi^-_{\nu j} . \tag{4}$$

The electronic wave functions $\psi'_{\mu j}(q_{\varkappa i})$ and the energies $E_{\mu j}(q_{\varkappa i})$ are now functions of the lattice distortions $q_{\varkappa i}$. The nuclear wave functions $\chi_k^{\mu j}(q_{\varkappa i})$ are eigenfunctions of $H_1 + E_{\mu j}(q_{\varkappa i})$, where k denotes the set of nuclear quantum numbers. The wave functions of the system are products of $\psi'_{\mu j}$ and $\chi_k^{\mu j}$ [10]:

$$\Psi_{\mu j}^k = \psi'_{\mu j} \chi_k^{\mu j} . \tag{5}$$

The oscillator strength f of the electronic dipole transition between the ground state ψ_0 and the excited state ψ'_μ is given by [10]

$$f_{0\mu} = \frac{2}{3} \frac{m^*}{\hbar^2} \bar{\varepsilon}_{0\mu} \, \mathrm{Av}_0 \sum_i \left| \langle \psi_0 | \sum_{j=1}^{z} \boldsymbol{r}_j | \psi'_{\mu i} \rangle \right|^2 . \tag{6}$$

m^* denotes the effective mass of the electron, $\bar{\varepsilon}_{0\mu}$ the mean energy of the transition, $\boldsymbol{r}_j$ the electric dipole operator, and Av_0 the thermal average over the ground state.

For the present we take only the linear term (3a) of H_{el} into account. We insert (4) into (6) and take the thermal average of products of the form $q_{\varkappa i} q_{\beta j}$. Since we consider static and dynamic distortions of the lattice cell, each ionic displacement $q_{\varkappa i}$ consists of a static part $Q_{\varkappa i 0}$ and a dynamic part $Q_{\varkappa i}$:

$$q_{\varkappa i} = Q_{\varkappa i} + Q_{\varkappa i 0} . \tag{7}$$

Using the orthogonality of the symmetry coordinates $q_{\varkappa i}$ of the complex we obtain

$$\begin{aligned} \langle q_{\varkappa i} q_{\beta j} \rangle &= \langle Q_{\varkappa i} Q_{\beta j} + Q_{\varkappa i} Q_{\beta j 0} + Q_{\varkappa i 0} Q_{\beta j} + Q_{\varkappa i 0} Q_{\beta j 0} \rangle = \\ &= \langle Q_{\varkappa i} Q_{\beta j} \rangle \delta_{\varkappa \beta} \delta_{ij} + Q_{\varkappa i 0} Q_{\beta j 0} . \end{aligned} \tag{8}$$

In analogy to the Jahn-Teller effect, the $Q_{\varkappa i 0}$ are the coordinates of the potential minima of the total energy of the complex including the linear electron–lattice interaction, but in contrast to the even-parity Jahn-Teller distortions, we only consider off-centre displacements with odd parity which do not contribute to the energy in first order. In linear approximation only distortions of odd parity contribute to the oscillator strength f of the transition. The octahedral complex has two threefold odd vibrations of Γ_4^--symmetry and one threefold degenerate odd vibration of Γ_5^--symmetry. Since IR resonance modes were observed in $NaCl:Cu^+$ and in $KCl:Ag^+$ we neglect effects from Γ_5^--modes and assume that only one Γ_4^--mode (q_{4i}^-) contributes to the parity breaking effect. $\boldsymbol{Q}_{40}^- = (Q_{4x0}^-, Q_{4y0}^-, Q_{4z0}^-)$ is called an off-centre distortion of the defect. We take the average of all the possible off-centre positions in the lattice cell:

$$\begin{aligned} \mathrm{Av(off\text{-}centre)} \; Q_{4i0}^- Q_{4j0}^- &= \frac{1}{N} \sum_{\text{off-c.}} Q_{4i0}^- Q_{4j0}^- = \\ &= Q_{4i0}^{2} \delta_{ij} = Q_{4j0}^{2} \delta_{ij} = \frac{1}{3} Q_0^2 \delta_{ij} . \end{aligned} \tag{9}$$