

《晶体中3d离子的光学性质》

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内容概要

《晶体中3d离子的光学性质:光谱和晶场分析(英文)》内容简介：The book is devoted to the analysis of spectral, vibronic and magnetic properties of 3d ions in a wide range of crystals, used as active media for solid state lasers and potential candidates for this role. crystal field calculations (including first-principles calculations of energy levels and absorption spectra) and comparison of these results with experimental spectra, jahn-teller effect, analysis of vibronic spectra, materials science applications are systematically dealt with. the chapters are relatively independent and can be read separately.

The book can be useful for researchers working in the areas of crystal spectroscopy, materials science and its optical applications, post-graduate and under graduate students.

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章节摘录

版权页：插图： The next consideration is about the vibrational modes of the ligands surrounding the SI. If, as above, we restrict to nearest neighbors in a tetrahedral environment we are left with a cage formed by the four anions, spanning 12 degrees of freedom. On the other hand the number of modes rapidly increases if one includes the next-nearest neighbors. Even worse, one should include all the vibrational modes of the host crystal making the problem quite intractable. To keep the state of affairs manageable some approximations are needed. The main point is that the SI are diluted and localized in the host crystal, the case to which we are here interested. Then one can assume a coupling of the electronic states to only one (or few) crystal lattice modes. In fact in this model, commonly adopted in the literature and quoted as cluster model (192) , a quasi molecular approximation is made assuming that only the vibrational motion of the impurity and its nearest neighbors (the cluster) can significantly influence the electronic state of interest. In this approximation the symmetrized normal coordinates of the quasi-molecule are taken as coordinates of the system and developed on the basis of the crystal phonon modes. Then it is assumed that there is only one mode (or few modes) whose expansion coefficients are predominate. Usually, different abundances in the phonons density of states of the host crystal may suggest the dominant mode as well as its energy and symmetry. At times, a second mode needs to be taken into consideration for a more precise description of the coupling. Another point to be discussed is related to the electric-dipole selection rules. As the reader has already noticed in the toy model discussed above, the electronic states are made with d functions. This character still remain after the CF splitting has come into play. The problem now is clear that electric-dipole transitions between the electronic multiplet E and T₂ are rigorously forbidden. The problem is beyond our toy model and origins from the dN configuration character of the electronic states. However, a deeper analysis shows that the Coulomb interaction in the free ion which weakly couples the 3d^N with other configurations at higher energy, thus making the electronic multiplet E and T₂ of indefinite parity and allowing for electric-dipole transitions between them. Finally, it should be noted that once vibrational coordinates enter the total Hamiltonian, the complete vibrational component should also form part of it on the same footing as the electronic component. It is usually considered that the vibrational Hamiltonian in the harmonic approximation which is justified by the low temperatures involved in the motivating experiments.

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编辑推荐

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