

Vibronic intensities in the electronic spectra of transition metal complex ions.
part x. second order herzberg-teller contributions to the vibronic intensity of the
4A_{2g} → 4T_{2g} transition in MnF₂ · 6H₂O

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A method to estimate the contribution to the vibronic intensity in electronic transitions of inorganic complex ions due to second order terms in the Herzberg-Teller expansion of vibronic wavefunctions is developed and applied to the 4A_{2g} → 4T_{2g} transition of the MnF₂ · 6H₂O ion. Both crystal field and ligand polarization contributions are derived, the crystal field term being evaluated in the single intermediate p state approximation. Contributions to the intensity of the nine second order terms are evaluated for several force fields and compared with recent experimental data. Although there are some difficulties in this comparison, it provides some support both for the model and the attribution of the intensity mechanism. © 1991 Taylor and Francis Group, LLC.