Vibronic intensities in centrosymmetric coordination compounds of the rare earths Part II. A vibronic crystal field-closure-ligand polarisation model and applications to the PrCl3-6 and UBr2-6 complex ions in octahedral symmetry

Acevedo, R.

Flint, C. D.

Meruane, T.

Muñoz, G.

Passman, M.

Poblete, V.

A symmetry adapted formalism to evaluate the vibronic intensities induced by the ungerade vibrational modes in centrosymmetric coordination compounds of the rare earths is put forward and applied to several selected electronic transitions of the PrCl3-6 and UCl2-6 complex ions in octahedral symmetry. This current model is based upon a modified symmetry adapted version of the combined vibronic crystal field-closure-ligand polarisation approach. This model differs from that developed in Part I of this series, in that for the vibronic crystal field contribution to the total transition dipole moment, the closure procedure is employed rather than the utilisation of a truncated basis set for the central metal intermediate electronic states. A criterion is introduced to choose an appropriate set of phases for both the electronic and the vibrational coordinates so that to ensure the right sign for the interference term (which couples together both the vibronic crystal field and the vibronic li