Vibronic intensities in the electronic spectra of transition-metal complex ions: Part VII. The ?8(2T2g) -> ?8(4A2g) electronic transition of the ReBr2-6 ion in Cs2ZrBr6

Acevedo, R.

Diaz, G.

Letelier, J. R.

Flint, C. D.

The vibronic intensities of the vibronic origins due to the three odd-parity vibrational modes of the ?8(2T2g) ?8(4A2g) electronic transition of the ReBr2-6 ion are calculated using both crystal-field and ligand-polarization vibronic models. The crystal-field calculations is carried out using the closure approximation, and both models employ the double-group formalism. The vibronic intensity distribution is different for the two models, but by using reasonable values of the radial integrals and atomic charges, satisfactory agreement with experiment is achieved.