Band shift in chromium (III) complexes with mixed ligands. A molecular orbital approach

Bunel, S.

Ibarra, C.

Adan, L.

The shift of the first and second spin allowed bands due to the stepwise replacement of the nitrogen atoms in a complex of Cr(III) of the CrN6 type by oxygen atoms of water or of carboxylic groups is analyzed in terms of perturbational molecule orbital theory. The set of parameters necessary to account for this effect has been obtained. Results agree fairly well with experimental data.