Auger Decay of Resonant Core-Excited (C 1s ® p*) States of CO_2

Katsuyuki Nobusada

Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, 060-0810, JAPAN

Auger decay of resonant core-excited (C 1s $\rightarrow$ π^*) states of CO_2 has been studied theoretically. To describe the intermediate excited states accurately, potential energy surfaces of the core-excited states as a function of symmetric stretch and bending motions are obtained by using ab initio calculations at the MCSCF (multi-configuration self-consistent-field) level of theory. As was pointed out in the studies of rough calculations based on the so-called Z+1 approximation, the present calculations show that the core excited state of $CO_2(1s^{-1}\ \pi^*)$ splits into two states depending on the bending motion (i.e., Renner-Teller splitting). π^* orbitals of the lower-energy state (A_1 state in C_{2v} molecular symmetry) lie in the bending plane and those of the higher-energy one (B_1 state) are out of that. To simulate the Auger decay spectra taking account of the coupling between the symmetric stretch motion and the bending one, we calculate the two-dimensional (symmetric stretch and bending) wave functions of the ground, intermediate, and final Auger states. The theoretical results will be compared with the recent experimental observations.