ELECTRONIC STRUCTURE OF GROUND AND SOME LOW-LYING EXCITED STATES OF CoCO: AN *AB INITIO* MOLECULAR ORBITAL STUDY

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MR-SDCI + Q and MR-ACPF molecular orbital calculations with the Roos-ANO basis sets have been carried out for the ground and some low-lying excited states of CoCO in order to determine the molecular constants and electronic structures, which will be comprehensive to those from the IR and millimeter-wave spectroscopies.[a] Dynamical electron correlations for the 8-10σ electrons are taking into account in the MR-SDCI + Q calculations with the active space consisting of Co $3d$, $4s$ orbitals and CO π, π^* orbitals. Relativistic energy corrections and spin-orbit interaction were also calculated. The electronic ground state was confirmed to be $^2\Delta_i$, and calculated rotational constant and vibrational frequencies agreed well with experimental values. Dipole moment and spin-orbit coupling constant were predicted to be 3.8 D and -486 cm^{-1}, respectively. Energy levels and electronic structure of some low-lying excited states have also been calculated.

[a]Hikida, *et al.*: two papers submitted to the session for Radicals and Ions of this 57th Symposium (2002).