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. 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 $^2\Delta_1$, 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.

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