THE PREDICTED INFRARED SPECTRUM OF THE HYPERMETALLIC MOLECULE CaOCa IN ITS LOWEST TWO ELECTRONIC STATES $\tilde{X}\ ^1\Sigma_g^+$ AND $\tilde{a}\ ^3\Sigma_u^+$

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This study of CaOCa is the third in a series by us on Group 2 alkaline-earth M_2O hypermetallic oxides. As with our previous calculations in the series, on BeOBe and MgOMg, the *ab initio* calculations we report here show that CaOCa has a linear $^1\Sigma_g^+$ ground electronic state and a very low lying linear $\tilde{a}\ ^3\Sigma_u^+$ first excited triplet electronic state. For CaOCa we determine that the singlet-triplet splitting $T_e(\tilde{a})$ = 386 cm^{-1}. We calculate the three-dimensional potential energy surface, and the electric dipole moment surfaces, of each of the two states using a multireference configuration interaction (MRCISD) approach in combination with internally contracted multireference perturbation theory (RS2C) based on full-valence complete active space self-consistent field (FV-CASSCF) wavefunctions with a cc-pwCVQZ-DK basis set for Ca and a cc-pCVQZ basis set for O. We simulate the infrared absorption spectra of $^{40}Ca^{16}O^{40}Ca$ in each of these electronic states in order to aid in its eventual spectroscopic characterization.