THE PREDICTED INFRARED SPECTRUM OF THE HYPERMETALLIC MOLECULE CaOCa IN ITS LOWEST TWO ELECTRONIC STATES $\tilde{X}\,^1\Sigma_\mathrm{g}^+$ AND $\tilde{a}\,^3\Sigma_\mathrm{u}^+$

B. OSTOJIĆ, *Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Studentski trg 14-16, 11 000 Belgrade, Serbia*; P. R. BUNKER, P. SCHWERDTFEGER, *Centre for Theoretical Chemistry and Physics (CTCP), The New Zealand Institute for Advanced Study(NZIAS), Massey University Auckland, Private Bag 102904, North Shore City, 0745 Auckland, New Zealand*; ARTUR GERTYCH, <u>PER JENSEN</u>, *FB C – Physikalische und Theoretische Chemie, Bergische Universität, D-42097 Wuppertal, Germany*.

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 $^1\Sigma_\mathrm{g}^+$ ground electronic state and a very low lying linear $\tilde{a}\,^3\Sigma_\mathrm{u}^+$ first excited triplet electronic state. For CaOCa we determine that the singlet-triplet splitting $T_\mathrm{e}(\tilde{a})$ = 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.