IONIZATION ENERGIES OF THE ISOMERS OF CN_2

JEREMY ARMSTRONG, LOVORKA DEGORICIJA, ANTHONY HILDEBRAND, JESSICA KOEHNE, and PATRICK E. FLEMING, *Department of Chemistry, Santa Clara University, 500 El Camino Real, Santa Clara, CA 95053*.

The geometries and harmonic vibrational frequencies for the structural isomers of CN_2 and the corresponding cations have been calculated at the B3LYP/6-311+g(2df) level. Adiabatic ionization energies were calculated at the G1, G2(MP2) and G2 levels as well for each of the isomers. Of the cations, the linear molecule CNN^+ is found to have the lowest energy. NCN^+ (also linear) lies 0.2 eV higher in energy than CNN^+. The other isomer of the cation, cyc-CN_2^+, has a cyclic structure with C_{2v} symmetry and lies 0.8 eV higher in energy than CNN^+. The adiabatic ionization energies of the radicals determined at the G2 level are IP(NCN) = 12.52 $\pm$ 0.07 eV, IP(CNN) = 11.01 $\pm$ 0.07 eV and IP(cyc-CN_2) = 11.94 $\pm$ 0.07 eV.