THE IONIZATION ENERGY OF THE DIAZOMETHYL (HCNN) AND CYANAMIDYL (HNCN) RADICALS

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The adiabatic ionization energy has been calculated for the diazomethyl radical (HCNN) and the cyanamidyl radical (HNCN) using ab initio methods. The B3LYP density functional method using the 6-311++g(3df,3pd)
basis set yields good results for the structures and vibrational frequencies of the radicals. The ionization energy is calculated using complete basis set extrapolation methods for both the radicals and associated cations. The lowest singlet and triplet states have been investigated for the cations. Results for the molecular structures and vibrational frequencies will be presented in addition to the calculated values of the ionization energies.