# THE $^2\Pi$ ELECTRONIC EXCITED STATES OF MgNC AND MgCN, AND THEIR SPECTROSCOPIC CONSTANTS

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MgNC is the first Mg-bearing molecule in space identified by us through the cooperative studies between *ab initio* molecular orbital calculations and the laboratory microwave study. We have extended the *ab initio* molecular orbital study to the first excited state $^2\Pi$ at the MR-SDCI/cc-pVTZ level of calculations. The vertical excitation energies of MgNC and MgCN, $^2\Pi$ - $^2\Sigma$, are 26289 and 23631 $cm^{-1}$, respectively. The $^2\Pi$ state equilibrium structures of MgNC and MgCN are found to be linear as are the case of their ground states. In contrast to the ground states, MgCN is more stable than MgNC by 2405 $cm^{-1}$. We also calculated A' and A" potential energy surfaces of the $^2\Pi$ state, and predicted spectroscopic constants therefrom. The calculated bending vibrational frequencies for the MgNC A' and A" surfaces were 120 and 160 $cm^{-1}$, respectively.