THE RENNER-TELLER EFFECT FOR THE $^2\Pi$ ELECTRONIC EXCITED STATE OF MgCN; AN *AB INITIO* MOLECULAR ORBITAL PREDICTION

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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[a] and the laboratory microwave study[b]. MgCN is its isomer, and has also been identified in space by Ziurys et al.[c] We have generated the potential energy surface of $^2\Pi$ electronic excited states of MgCN at the MR-SDCI/aug-cc-pVQZ level of calculations, and predicted spectroscopic constants. The potential energy surface shows that MgCN has a linear structure in the $^2\Pi$ electronic state, which splits into two states, $^2A'$ and $^2A"$ via Mg-C-N bending motions (Renner-Teller splitting). The Renner parameter ϵ is calculated as 0.24 for $^2\Pi$ in MgCN, which is smaller than the corresponding value for $^2\Pi$ in MgNC (ϵ = 0.32).

[a]K. Ishii, T. Hirano, U. Nagashima, B. Weis, and K. Yamashita, *Astrophys. J.* **410**, L43, (1993)
[b]K. Kawaguchi, E. Kagi, T. Hirano, S. Takano, and S. Saito, *Astrophys. J.* **406**, L39, (1993)
[c]L. M. Ziurys, A. J. Apponi, M. Guelin, and J. Cernicharo *Astrophys. J.* **445**, L47, (1995)