AB INITIO MOLECULAR ORBITAL CALCULATIONS OF SPECTROSCOPIC CONSTANTS OF SOME ASTRONOMICALLY INTERESTING MOLECULES: MgNC, MgCN, CaNC, CaCN, AND FeCO

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To assist the laboratory identification[a] of the first Mg-bearing interstellar molecule MgNC, we carried out *ab initio* molecular orbital calculations of the spectroscopic constants of $X\ ^2\Sigma^+$ MgNC and MgCN by the SDCI (frozen core)/TZ2P method as is described in our previous papers.[b] This time, we calculated potential energy surfaces (PES) of $X\ ^2\Sigma^+$ states of MgNC and MgCN by the CASSCF-ACPF/TZ2P+f method with core-valence electron correlation, and derived spectroscopic constants therefrom. Calculated rotational constant B_0, centrifugal distortion constant D_0, and vibration frequencies ω_1, ω_2, and ω_3, with corresponding experimental values for MgNC[a] and for MgCN[c] in parentheses, are 5969.3 (5966.8969) MHz, 0.0029 (0.0042) MHz, and 2097.9, 90.4 (86), and 538.5 cm^{-1} for MgNC, and 5089.3 (5094.80351) MHz, 0.0025 (0.00277) MHz, and 2177.2, 159.9, and 468.6 cm^{-1} for MgCN, respectively. Great improvement resulted from the inclusion of core-valence electron correlation. Similar calculations have been carried out for CaNC and CaCN, where the inclusion of both core-core electron and core-valence electron correlations is found to be very important. While the PES for the ground state CaCN is quite normal and shallow, the PES for the ground state CaNC is shallow but of very complicated character. The predicted B_0 of CaNC is 3982.8 MHz against the experimental value[d] of 4048.742 MHz. Preliminary calculations for B_e of FeCO have also been carried out.

[a] K. Kawaguchi, et al., Astrophys. J. 406, L39 (1993).
[b] K. Ishii, et al., Astrophys. J. 410, L43 (1993); K. Ishii, et al., THEOCHEM, 305, 117 (1994).
[c] M.A. Anderson, et al., Astrophys. J., 429, L41 (1994).
[d] T.C. Steimle, et al., Astrophys. J, 410. L49 (1993).