AN *AB INITIO* MOLECULAR ORBITAL STUDY ON THE STRUCTURE AND SPECTROSCOPIC PROPERTIES OF MAGNESIUM DICARBIDE

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A magnesium-bearing molecule MgC_2 is one of the candidate to be found in the envelope of a carbon star. Element magnesium may be rich in astrophysical objects because the elemental cosmic abundance of magnesium and silicon is almost the same, while silicon containing molecules such as SiO, SiS, SiC, SiC_2, SiC_4, SiH_4, SiN, have been found in interstellar space. Silicon dicarbide SiC_2 was discovered in IRC+10216. Now, magnesium dicarbide, MgC_2, is strongly expected to be observed. Since none of the experimental spectroscopic data on MgC_2 has been reported in any frequency region, *ab initio* molecular orbital predicition has been requested for its identification.

The MR-SDCI+Q calculations with augmented cc-pVQZ basis sets have predicted that the ground state MgC_2 ($^1A_1$) has T-shaped structure of C_{2v} symmetry consisting of Mg^+ cation and CC^- moiety with the dipole moment of 7.9 Debye. The CC and MgC distances have been found to be 1.275 and 2.012 Å in its equilibrium geometry.

The MR-SDCI+Q three-dimensional potential energy surface consisting of 497 points were analysed by the 2nd-order perturbation theory, predicting the rotational constants A_0, B_0, and C_0 to be 51794.0, 11493.9 and 9378.7 MHz, and the centrifugal distortion constants $\Delta_J, \Delta_{JK}, \Delta_K, \delta_J, \delta_K$ to be 0.014, 0.21, -0.023, 0.0027, 0.14 MHz, respectively. The ν_1(CC stretching), ν_2(Mg-C_2 streching), and ν_3(bending) vibrational frequencies have been estimated to be 1704.2, 594.8 and 455.8 cm^{-1}, respectively. These results indicate that MgC_2 molecule is a rigid molecule unlike the analogue SiC_2, which is known as a molecule with large-amplitude motion. Toward the laser induced fluorescent spectroscopy, the vertical excitation energies for $\tilde{A}\,^1A_1 \leftarrow \tilde{X}\,^1A_1$ and $\tilde{B}\,^1B_2 \leftarrow \tilde{X}\,^1A_1$ trasitions have also been calculated to be 8334 and 13034 cm^{-1}, respectively, at the CAS-SCF level of theory.