STABILITY AND SPECTROSCOPY OF MO_2 METAL DIOXIDES, M=B, Al, Ga, In, Tl

N. TERZI, , *Laboratoire de Spectroscopie Atomique Moléculaire et Applications, Faculté des Sciences de Tunis, Université Tunis El Manar, Tunis*

By making use of both theories, Wave Funcion Theory with Cluster Coupled (CCSD(T)) method and Functional Density Theory with B3LYP functional, we have performed geometry optimization of metallic dioxide molecules, metal belongs to the 13th column of the periodic table. Wave functions are expressed using respectively, Dunning, Pople and Los Alamos basis sets, aug−cc−pvtz, aug−cc−pwcvnz (nz = tz, qz, 5z), 6−311++G** and Lanl2DZ. Geometrical parameters as well as infrared spectra are reported for all optimized geometries. Molecular orbitals for the most stable structures are given as well [1]. Our calculations indicate that there are five possible isomers with linear or folded shapes. Some discrepancies with previous results are also noted. It is worth mentioning that there is a good agreement of geometry parameters obtained at two levels of theory when using awcvqz−pp and awcv5z−pp bases sets. It was possible to identify the good agreement between our CCSD(T)/awcvqz−pp, awcv5z−pp and B3LYP/Lanl2DZ spectroscopic results and experimental available values [2] [3]. A spectroscopic study and NBO analysis, were devoted to explain the relative stability of the $^2A_2$ structure compared to $^2A_1$ one, in both cases of AlO_2 and GaO_2 systems, and its absolute stability in both cases InO_2 and TlO_2 molecules. We concluded that $^2A_2$ owes its stability to its ionic structure planned by the Russian experimenters [4].

[1] N. Terzi, S. Hosni, Y. Arfaoui, Computational and Theoretical Chemistry 1213, 113730 (2022)
[2] J. Johns, Canadian Journal of Physics 39(12), 1738 (1961)
[3] A. Köhn, B. Gaertner, H.J. Himmel, Chemistry−A European Journal 11(19), 5575 (2005)
[4] L. Serebrennikov, S. Osin, A. Maltsev, Journal of Molecular Structure 81(1−2), 25 (1982)

p-number: p002 **Submitted on Wed, 10 May 2023 23:23:17 +0200**