ELECTRONIC STRUCTURE AND SPECTROSCOPY OF THE MgO_2^+ CATION

O. YAZIDI, A. BEN HOURIA AND Z. BEN LAKHDAR, *Laboratoire de Spectroscopie Atomique, Moléculaire et Applications-LSAMA, Université de Tunis El Manar, Tunis, Tunisia.*; M. HOCHLAF, *Université Paris-Est, Laboratoire de Modélisation et Simulation Multi Echelle (FRE 3160 CNRS), Champs sur Marne, F-77454 Marne-la-Vallée, Cedex 2, France.*; M.L. SENENT, *Departamento de Astrofísica Molecular e Infrarroja, Instituto de Estructura de la Materia, C.S.I.C., Madrid 28006, Spain..*

Highly correlated *ab initio* methods are used to investigate the lowest MgO_2^+ electronic states. Our computations confirm the existence of the strongly bent (MgO_2^+ X^2 A_2) form and the weakly bound *l*-MgOO^+ (X^4 Σ^-) charge quadrupole complex [a].
For both isomers, the three-dimensional potential energy surfaces ($3D - PESs$) of their electronic ground states are mapped in internal coordinates not far from their respective equilibrium geometries. Then a set of spectroscopic parameters are derived using second order perturbation theory. The rovibrational spectra are also deduced variationally. One-dimensional cuts of the $3D - PESs$ of the lowest doublet and quartet electronic states of MgO_2^+ along the R_{MgO} and R_{OO} stretching and bending coordinates, are calculated, covering both the molecular ans the asymptotic regions. These curves are used later in order to discuss the metastability of these electronic states and to propose mechanisms for the Mg^+ + O_2 atmospheric ion-molecule reaction. [b].

[a] M. Sodupe and C.W. Bauschlicher, Jr., *Chem.Phys.Lett.*, **203**, 215 (1993)
[b] O. Yazidi, A. Ben Houria, Z. Ben Lakhdar, M.L. Senent and M. Hochlaf (submitted, 2008)