Characterisation of The Ground and Low-Lying Excited States of MgO^+ by PFI-ZEKE Photoelectron Spectroscopy

J. R. Schmitz[1], C. Kreis[1], F. Merkt[1]*

[1]Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich, Switzerland

We report on the characterisation of the rovibrational structure of the ground and first excited electronic states of MgO^+ by high-resolution pulsed-field ionization zero-kinetic-energy (PFI-ZEKE) photoelectron spectroscopy. Rotationally cold (T_{rot}=5 K) MgO molecules in the X $^1\Sigma^+$ (v = 0-2) levels were generated in a supersonic expansion of a 0.1% N_2O:He gas mixture following laser ablation off a magnesium (Mg) rod [1]. The rovibrational ionization thresholds corresponding to both spin-orbit components (Ω=1/2, 3/2) of the $X^+\ ^2\Pi_\Omega$ (v^+ = 0-10) states as well as to the first excited $A^+\ ^2\Sigma^+_{1/2}$ (v^+ = 0-10) state were reached in a resonant 1+1' two-photon excitation sequence via the rovibrational levels of the F $^1\Pi$, E $^1\Sigma^+$, G $^1\Pi$ and 3 $^3\Pi_2$ intermediate levels of MgO studied previously by Breckenridge and coworkers [2, 3]. Our new results include accurate values for the adiabatic ionization energy of MgO and for the dissociation energies of the MgO X $^1\Sigma^+$ and MgO^+ $X^+\ ^2\Pi_\Omega$ and $A^+\ ^2\Sigma^+_{1/2}$ states. This work is carried out in the context of our studies of the rovibrational structure of doubly charged dications by high-resolution PFI-ZEKE spectroscopy of singly-charged cations following the approach recently taken to characterise the ground state of the thermodynamically stable dication $MgAr^{2+}$ [4]. The talk will present a roadmap towards characterising the ground state of MgO^{2+} by resonant multiphoton excitation via electronically excited states of MgO^+. The experiments will reveal whether MgO^{2+} is thermodynamically stable as predicted in Ref. [5] or metastable as predicted in Ref. [6].

[1] Thomas D. Persinger, Daniel J. Frohman, Wafaa M. Fawzy, Michael C. Heaven, *J. Phys. Chem.,* **2020,** 153, 054308.
[2] Jinjin Wang, W.H. Breckenridge, *J. Chem. Phys.,* **2006,** 124, 124308.
[3] D. Bellert, Katherine L. Burns, Nguyen-Thi Van-Oanh, Jinjin Wang, W.H. Breckenridge, *Chem. Phys. Lett.,* **2003,** 381, 381-384.
[4] Dominik Wehrli, Matthieu Génévriez, Frédéric Merkt, *Phys. Chem. Chem. Phys.,* **2021,** 23, 10978-10987.
[5] R. Linguerri, M. Hochlaf, M.-C. Bacchus-Montabonel, M. Desouter-Lecomte, *Phys. Chem. Chem. Phys.,* **2013,** 15, 24-831.
[6] Marcin Kolbuszewski, James S. Wright, *Chem. Phys. Lett.,* **1994,** 218, 338-342.