

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

J. R. Schmitz¹, C. Kreis¹, F. Merkt^{1*}

¹Department 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 ($T_{\text{rot}}=5$ K) MgO molecules in the $X^1\Sigma^+$ ($v = 0-2$) levels were generated in a supersonic expansion of a 0.1% $\text{N}_2\text{O}:\text{He}$ gas mixture following laser ablation off a magnesium (Mg) rod [1]. The rovibrational ionization thresholds corresponding to both spin-orbit components ($\Omega=1/2, 3/2$) 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 $\text{MgO } X^1\Sigma^+$ and $\text{MgO}^+ X^+ 2\Pi_{\Omega}$ 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.