## Abstract Submitted for the DAMOP09 Meeting of The American Physical Society

New determination of the structure parameters in the molecular tunneling ionization model SONG-FENG ZHAO, CHENG JIN, ANH-THU LE, CHII-DONG LIN, Kansas State University — Molecular ADK model (MO-ADK) [1] has been successfully used to study the ionization of molecules in recent years. However, there is indication that the model does not predict the correct alignment dependence of the ionization rates for CO<sub>2</sub> molecules [2]. In the MO-ADK model, the wavefunction of the highest-occupied orbital at large distance is needed in the tunneling region. The wavefunction calculated using the quantum chemistry code usually is not accurate at large distance. In this work, we re-examined the MO-ADK model where the HOMO wavefunction are calculated using B-splines functions in the one-center expansion. Results from the MO-ADK models for several molecules will be presented and compared to those from other ab initio calculations whenever available. [1] X. Tong et al, Phys. Rev. A 66, 033402(2002). [2] D. Pavicic et al, Phys. Rev. Lett. 98, 243001 (2007).

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