## Abstract Submitted for the DAMOP16 Meeting of The American Physical Society

Near-Threshold, Vibrationally-Resolved Photoionization of Molecular Nitrogen GAETAN VANGYSEGHEM, THOMAS GORCZYCA, Western Michigan University, CONNOR BALLANCE, Queen's University Belfast — Photoionization of molecular nitrogen  $(N_2)$  is investigated near the first ionization threshold using an R-matrix, multi-channel quantum defect theory (MQDT) approach. Building on an existing fixed-nuclei R-matrix photoionization model [M. Tashiro, J. Chem. Phys. 132, 134306, (2010)], which, in turn, is built on the UKRmol suite of codes, photoionization cross sections, as well as scattering and dipole matrices, are computed in the Born-Oppenheimer approximation. By varying the internuclear separation, potential energy curves have been constructed for the  $N_2$  and  $N_2^+$  states and compared to quantum chemistry calculations. Using these fixed-nuclei potential energy curves, and corresponding vibronic eigenenergies and eigenfunctions, a frame transformation is enacted on the fixed-nuclei scattering and dipole matrices, allowing for the calculation of vibrationally-resolved photoionization cross sections. The resultant photoionization cross sections are compared to highresolution experimental data [P. O'Keeffe et al. J. Chem. Phys 136, 104307, (2012)] near threshold, a region complicated by multiple vibrationally-resolved, interacting Rydberg series.

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