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Near-Threshold, Vibrationally-Resolved Photoionization of Molecular Nitrogen GAETAN VANGYSEGHM, THOMAS GORCZYCA, Western Michigan University, CONNOR BALLANCE, Queen's University Belfast — Photoabsorption of molecular nitrogen (N_2) is investigated near the first ionization threshold using an R-matrix, multi-channel quantum defect (MQDT) approach. Building on an existing fixed-nuclei R-matrix photoionization model [M. Tashiro, J. Chem. Phys. 132, 134306, (2010)], single and multiple configuration molecular descriptions have been considered using the UKRmol suite of codes. Photoionization cross sections, as well as reactance and dipole matrices, are first computed in the fixed-nuclei approximation. The smooth eigenquantum defects are parameterized as a function of electron scattering energy and internuclear separation for further MQDT rovibrational frame transformation calculations. Potential energy curves for the N_2 and N_2^+ states have also been constructed in order to assess the accuracy of the molecular structure. Comparison with high-resolution experimental photoionization cross sections is also made near threshold, a region complicated by multiple vibrationally-resolved, interacting Rydberg series.

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