AB INITIO AND EMPIRICAL STUDIES OF ELECTRONICALLY EXCITED STATES OF PHOSPHOROUS MONONITRIDE (PN) AND ITS ROVIBRONIC SPECTROSCOPY

MIKHAIL SEMENOV, *Department of Physics and Astronomy, University College London, London, UK*; NAYLA EL-KORK, *Physics, Khalifa University, Abu Dhabi, United Arab Emirates*; SERGEI N. YURCHENKO, JONATHAN TENNYSON, *Department of Physics and Astronomy, University College London, London, UK*.

We report an *ab initio* study on the rovibronic spectroscopy of the open-shell diatomic molecule phosphorous mononitride, PN. The study considers nine lowest electronic states, $X^1\Sigma^+$, $A^1\Pi$, $C^1\Sigma^-$, $D^1\Delta$, $E^1\Sigma^-$, $a^3\Sigma^+$, $b^3\Pi$, $d^3\Delta$ and $e^3\Sigma^-$, using high level electronic structure theory and accurate nuclear motion calculations. Using the *ab initio* data for bond lengths ranging from 1 to 3.16Å, we compute 9 potential energy, 9 spin-orbit coupling, 7 electronic angular momentum coupling, 9 electric dipole moments, and 9 transition dipole moment curves. The Duo nuclear motion program [a] is used to solve the coupled nuclear motion Schrödinger equations for these nine electronic states. The spectra of $^{31}P^{14}N$ simulated for different temperatures are compared with several available high-resolution experimental studies. Lifetimes are calculated for all states and reported here with comparison to previous results in the literature. We then produce a separate line list for the $X^1\Sigma^+$, $A^1\Pi$, $E1\Sigma^-$ states, with the potential energy functions and some couplings being fitted the experimental energy values inverted using the MARVEL procedure.

[a] S. N. Yurchenko, L. Lodi, J. Tennyson, A. V. Stolyarov, *Comput. Phys. Commun.*, 2016, **202**, 262 – 275; see *https://github.com/exomol*.