EXOMOL ROVIBRONIC LINE LIST AND TEMPERATURE DEPENDENT PHOTODISSOCIATION CROSS SECTION CALCULATIONS FOR OH FROM *AB INITIO* ELECTRONIC STRUCTURE CALCULATIONS

GEORGI B MITEV, JONATHAN TENNYSON, SERGEI N. YURCHENKO, *Department of Physics and Astronomy, University College London, London, UK*.

OH spectroscopy has been heavily studied due to its importance in combustion, atmospheric and interstellar chemistry, and as a key constituent of the Earth's atmosphere. Recently, OH has been detected in the atmosphere of the Ulta-Hot Jupiter WASP-76b and has also been found in the stellar spectra of M-dwarfs[a]. Novel MolPro electronic structure calculations for ground and excited electronic state PECs will be presented along with associated coupling curves and (transition) dipole moments. These *ab initio* calculations are used to produce a ExoMol rovibronic linelist using the programs Duo and ExoCross. Photodissociation is a primary destructor of OH in diffuse interstellar clouds, particularly the direct $X\ ^2\Pi \rightarrow\ 1^2\Sigma^-$ photodissociation. $A\ ^2\Sigma^+$ predissociation is also studied. Temperature-dependent photodissociation cross sections using the method established by Pezzella et al.[b] are calculated and presented. Gaussian line profile optimization of photodissociation cross sections has been automated and applied to the cases of direct photodissociation for OH, HCl, and HCN.

---

[a]R. Landman, A. Sánchez-López, P. Mollière, A. Y. Kesseli, A. J. Louca, I. A. G. Snellen, *A&A*, 2021, **656**, A119

[b]M. Pezzella, J. Tennyson, S. N. Yurchenko, *Phys. Chem. Chem. Phys.*, 2021, **23**, 16390