IMPROVING THE ROTATION VIBRATIONAL LINE LISTS FOR OZONE

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There are long running problems over the precise transition intensities and line positions for ozone[a,b]. In our work, state of the art, first principles quantum mechanical methods are being used to compute high accuracy transition intensities and line positions for the microwave and infrared regions of the spectrum of ozone. In this presentation I will discuss details of our most recent calculations of the ab initio dipole moment surface (DMS) and analysis of experimental ozone line positions using the MARVEL (Measured Active Rotation Vibration Energy Levels) technique[c]. To improve the quality of our current[d] DMS we are exploring the electronic structure model, finer grids and larger basis set sizes. The ozone MARVEL project currently involves the analysis of around 70 sources of scientific literature (we anticipate this number to increase). We will use the MARVEL energy levels to fit a new potential energy surface for ozone. We also intend to replace the calculated energy levels with MARVEL energy levels in our line lists. We hope the results of this study will be important for a range of atmospheric studies, such as self-consistency of ozone concentration retrievals in remote sensing techniques, and possible detections of ozone in exo-planetary atmospheres.

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[b] A. Barbe et al, "Ozone spectroscopy in the electronic ground state: High-resolution spectra analyses and update of line parameters since 2003", Journal of Quantitative Spectroscopy and Radiative Transfer, **130**, 172–190 (2013)

[c] T. Furtenbacher, A. G. Császár & J. Tennyson, "MARVEL: measured active rotational–vibrational energy levels.", Journal of Molecular Spectroscopy, **245**, 115–125 (2007)

[d] O. L. Polyansky, N. F. Zobov, I. I. Mizus , A. A. Kyuberis, L. Lodi & J. Tennyson, "Potential energy surface, dipole moment surface and the intensity calculations for the 10 μm, 5 μm and 3 μm bands of ozone", Journal of Quantitative Spectroscopy and Radiative Transfer, **210**, 127–135 (2018)