SPECTROSCOPIC MODEL AND PREDISSOCIATION LIFETIMES OF THE HYDROXYL RADICAL

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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. It is found in planetary atmospheres, comets, stellar atmospheres and interstellar clouds. Furthermore, recently OH has been detected in the atmospheres of Ultra-hot Jupiters WASP-76b and WASP-33b.[1,2]

Novel multi-reference configuration interaction calculations for the X $^2\Pi$, A $^2\Sigma^+$, 1 $^2\Sigma^-$, 1 $^4\Sigma^-$, and 1 $^4\Pi$ potential energy curves (PECs), associated coupling curves and (transition) dipole moments are presented. Curves are refined against empirical energy levels and transitions from the latest MARVEL OH data[3] using the bound state nuclear motion code Duo [4].

The effect of predissociation of the A $^2\Sigma^+$ energy levels caused by a spin-orbit interaction with with repulsive (unbound) electronic states $^2\Sigma^-$ and $^4\Sigma^-$, $^4\Pi$ is studied. Predissociation is one of the the main sources of line broadening of the A–X rovibronic transitions.

In Duo, continuum states are treated as bound states by adding infinite potential barriers to the unbound PECs at the long-range boundary defined by the internuclear distance (R_c). Varying R_c allows us to scan continuum states, giving a series of crossings between (quasi) bound states associated with the A $^2\Sigma^+$ and continuum states, from which we are able to extract spin-orbit induced predissociation lifetimes with good agreement to experimental data.

Python package, **binSLT**, a parallelised code to calculate predissociation lifetimes, associated line broadening parameters, and uncertainties from Duo *.states files are presented and will be available on the ExoMol GitHub. The potential energy and other curves from this study will be used to produce a rovibronic ExoMol linelist and temperature dependent photodissociation cross sections for the for hydroxyl radical.

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[1] doi: 10.1051/0004-6361/202141696, R. Landman et al. Detection of OH in the ultra-hot Jupiter WASP-76b, A&A 656, A119 (2021)

[2] doi: 10.48550/arXiv.2305.11071 O. Wright et al. A spectroscopic thermometer: individual vibrational band spectroscopy with the example of OH in the atmosphere of WASP-33b, A&AS, in press (2023).

[3] doi: 10.1039/D2CP02240K, T. Furtenbacher, S. T. Hegedus, J. Tennyson, A. G. Császár, Analysis of measured high-resolution doublet rovibronic spectra and related line lists of ^{12}CH and ^{16}OH, Phys. Chem. Chem. Phys. 24, 19287 (2022)

[4] doi: 10.1016/j.cpc.2015.12.021, S. N. Yurchenko, L. Lodi, J. Tennyson, A. V. Stolyarov, Duo: A general program for calculating spectra of diatomic molecules, Comp. Phys. Comm., 202, 262 (2016), https://github.com/exomol/duo