

ExoMol photodissociation cross-sections – V. Photodissociation rates of the SO radical

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Accepted 2026 July 13. Received 2026 July 9; in original form 2026 May 1

ABSTRACT

Rovibronic state-resolved predissociation rates and temperature-dependent photodissociation cross-sections are computed for sulphur monoxide ($^{32}\text{S}^{16}\text{O}$). We present a refinement of the ExoMol SOLIS spectroscopic model using empirical (MARVEL) rovibronic energy levels for the $B^3\Sigma^-$ and $C^3\Pi$ states. To accurately model predissociation, the lowest quintet state, $(1)^5\Pi$, and its associated couplings are incorporated, with line widths determined via a stabilization approach. The total photodissociation cross-sections account for both direct photoabsorption and predissociation. To ensure completeness, a short-wavelength ‘top-up’ from the Leiden data base is integrated for regions where the current model does not capture specific predissociation coupling mechanisms. Our results demonstrate that SO photodissociation rates are highly sensitive to temperature; for instance, under a 3000 K blackbody radiation field, rates vary by three orders of magnitude across the molecular temperature range studied. The new SOLUVIS cross-sections are available via the ExoPhoto data base <https://www.exomol.com/ExoPhoto>.

Key words: molecular data – molecular processes – exoplanets – photodissociation region (PDR) – ultraviolet: general.

1 INTRODUCTION

Photochemistry has a profound influence on the molecular composition and thermal dynamics of astronomical environments exposed to intense ultraviolet (UV) radiation fields. A critical photochemical process is photodissociation, where the absorption of high-energy photons leads to the fragmentation of molecules either through direct excitation into the continuum or via short-lived states that transition to the continuum through various mechanisms (G. Herzberg 1939). In UV-rich environments, this process directly disrupts chemical equilibrium since molecules fragment into reactive species and populate excited rovibronic states that drive the medium far from local thermodynamic equilibrium (LTE). While established repositories like the Leiden data base (A. N. Heays, A. D. Bosman & E. F. van Dishoeck 2017; H. R. Hrodmarsson & E. F. Van Dishoeck 2023) have provided an invaluable foundation for modelling cold environments such as the interstellar medium (ISM), these data sets assume molecules reside exclusively in their ground vibronic states and thus their photodissociation data are suitable only for $T = 0$ K (in some cases room temperature). This is an issue, however, for studying astrophysical objects at higher temperatures. For example, temperatures frequently exceed 1000 K in exoplanets orbiting in close proximity to their host stars. In these high-temperature regimes, the population of excited rovibrational states significantly alters

photodissociation cross-sections, sometimes by orders of magnitude (M. Pezzella, S. N. Yurchenko & J. Tennyson 2022), driving the system far from LTE. Because photodissociation drives non-LTE chemistry, relying on cold-molecule data can lead to inaccuracies in chemical equilibrium and atmospheric dynamics modelling of these objects. To ensure the reliability of atmospheric retrievals and the interpretation of high-resolution spectra, it is essential to study the temperature-dependent photodissociation for the molecules of interest. This work aims to address this data gap by providing temperature-dependent photodissociation rates and cross-sections for Sulphur monoxide (SO).

SO is observed across a vast range of environments, from terrestrial combustion and volcanic plumes to the ISM. As a key intermediate in the oxidation of sulphur compounds, SO is central to atmospheric chemistry, contributing to acidification of terrestrial rain and atmospheric pollution through its high reactivity with N_2 and O_2 (A. G. Gaydon 1948; J. B. Burkholder et al. 1987; M. Wang 2004; G. D. Thurston 2017; X. Pan 2019, 2011). Astrophysically, SO holds historical significance as the first $^3\Sigma^-$ ground-state molecule detected in the ISM via rotational spectroscopy (C. A. Gottlieb & J. A. Ball 1973) and the first to be observed in excited electronic states using microwave spectroscopy (S. Saito 1970). It has since been identified in interstellar and molecular clouds (C. A. Gottlieb & J. A. Ball 1973; C. A. Gottlieb et al. 1978; G. A. Blake et al. 1987; C. Codella & D. Muders 1997), protoplanetary discs (S. Pacheco-Vazquez et al. 2015; T. H. G. Vidal et al. 2017; J. C. Laas & P. Caselli 2019), protostellar environments (M. N. Drozdovskaya et al. 2018; A. Garufi et al. 2022;

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A. Dutrey et al. 2024), and various solar system bodies, including the atmospheres of Venus and Jupiter’s moon Io (C. Y. Na, L. W. Esposito & T. E. Skinner 1990; E. Lellouch 1996; I. de Pater et al. 2002; D. A. Belyaev et al. 2012). Given its role in sulphur-carrier dust formation (T. H. G. Vidal et al. 2017; J. C. Laas & P. Caselli 2019) and its prevalence in volcanic planetary atmospheres (M. Y. Zolotov & B. J. Fegley 1998; V. A. Krasnopolsky 2012; R. Hobbs et al. 2021), SO is an essential tracer for understanding both the chemical evolution of exoplanetary systems and the dynamics of planetary formation.

SO is now expected to be present in regions where photochemistry is important. A recent example is the detection of SO₂ in the atmosphere of the hot-Jupiter WASP-39b (Z. Rustamkulov et al. 2023; S.-M. Tsai et al. 2023b), which established SO as an intermediate in the photochemical pathways of sulphur chemistry in the atmosphere. This discovery marked a major milestone – the first clear observation of UV-driven sulphur photochemistry in a hot exoplanet which was only possible by including photodissociation in the chemical modelling and subsequent atmospheric retrievals. To validate the conclusions in these works, it is essential to determine the temperature dependence of the photodissociation processes in the relevant sulphur bearing molecules in the photochemical pathways. Indeed, the broader atmospheric modelling community has increasingly recognized this necessity, driving significant experimental efforts to measure high-temperature cross-sections for other key atmospheric species (e.g. CO₂; O. Venot et al. 2018). To the best of our knowledge, the only available photochemical data for SO, such as those provided by the Leiden data base, rely on the single temperature measurements of L. F. Phillips (1981) and A. N. Heays et al. (2022), the latter providing some temperature dependent semi-empirical models. In this study, we aim to refine current photochemical models by providing the first temperature-dependent photodissociation cross-sections and rates for SO. We utilize the methodology developed by ExoMol (M. Pezzella, S. N. Yurchenko & J. Tennyson 2021), incorporating a significant update to the SOLIS spectroscopic model (R. P. Brady et al. 2023) in a new hybrid SO line list called SOLUVIS and a set of photodissociation cross-sections for which we use the same model.

2 METHODOLOGY

The predominant predissociated UV absorption bands of SO between 190 and 235 nm, identified as the $B^3\Sigma^- - X^3\Sigma^-$ transition, were previously measured by L. F. Phillips (1981). Our *ab initio* SO spectrum (R. P. Brady et al. 2022) confirms that this band is orders of magnitude stronger than any overlapping electronic transitions in this region (with the exception of the $A^3\Pi - X^3\Sigma^-$ band between $\sim 38\,000 - 40\,000\text{ cm}^{-1}$). While J. B. Nee & L. C. Lee (1986) reported absorption within the far-ultraviolet (FUV) range (116–135 nm), these features are not currently covered by our spectroscopic models. To ensure completeness, we have supplemented our cross-sections using this experimental data; details of which are discussed in Section 4.1.

The following section describes the spectroscopic models and methodologies employed to determine the predissociation rates for the $B^3\Sigma^-$ and $C^3\Pi$ electronic states, which we, experiment (L. F. Phillips 1981; A. N. Heays et al. 2022), and theory (C.-P. Liu et al. 2006; L. Yu & W. Bian 2011; K. Sarka & S. Nanbu 2019) identify to be the important states for computing the (temperature dependent) photodissociation rates of SO.

2.1 Nuclear motion calculations

DUO (S. N. Yurchenko et al. 2016) is a general-purpose (open access¹) variational code for solving the rovibronic Schrödinger equation of diatomic molecules. It constructs a spectroscopic model by incorporating arbitrary couplings between electronic states, including (but not limited to) spin-orbit, electronic angular momentum, and spin-rotational terms. Typically, electronic property curves such as potential energy curves (PECs), spin-orbit couplings (SOCs), electronic angular momentum couplings (EAMCs), and (transition) dipole moment couplings ((T)DMCs) are computed *a priori* using quantum chemistry packages like MOLPRO (H.-J. Werner et al. 2012) under the Born–Oppenheimer approximation. DUO represents these as either analytical functions or grids mapped via cubic splines. Nuclear motion is solved using the sinc-DVR method (R. Guardiola & J. Ros 1982; J. R. Lund & B. V. Riley 1984) to first build a vibrational basis in which the rovibronic Hamiltonian is constructed in a Hund’s case (a) basis to obtain eigenstates and energies for total angular momentum J and parity. Other quantum numbers are assigned by the largest basis set coefficient. Using these eigenfunctions, DUO computes transition line strengths, Einstein A coefficients, and radiative lifetimes. Output includes a .STATES file (energy and quantum numbers) and a .TRANS file (transition frequencies and A coefficients).

In variationally solving for the vibronic energies with the sinc-DVR method, DUO introduces a potential barrier of infinite height at the ‘right hand’ side of the simulation region at bond length L_{max} ; the so-called particle in a box problem. This is synonymous with the boundary condition where eigenstate wavefunctions and their derivative with bond length, r , are set to zero at the simulation border. Whilst this methodology is sufficient for solving bound rovibronic states which come as solutions to the nuclear motion inside potential wells (where the wavefunctions exponentially decay outside the potential), it does not provide a complete solution to the continuum region where states are unbound (such as those for electronic states which are repulsive, see Fig. 1). Since we introduce a finite simulation box size, the continuum is truncated to the solutions which satisfy the boundary conditions, consequently the continuum is effectively discretized. This means that computing proper continuum coupling to bound-states, which leads to their quasi-bound character, is not reconstructed in a single calculation. Since DUO solves the time-independent diatomic Schrödinger equation without complex absorbing potentials, the broadening of quasi-bound rovibronic states due to the continuum is then reconstructed statistically through a stabilization procedure detailed in Section 2.6.

2.2 Bound and unbound solutions

In order to compute continuum photoabsorption and bound-(quasi)bound cross-sections, they need to be treated separately. We then separate our DUO bound and unbound solutions of nuclear motion. Unbound states can be identified if their wavefunctions oscillate with large amplitude at large bond lengths, whereas bound states have exponentially decaying tails and approach zero for $r \rightarrow L_{\text{max}}$. An amplitude filter, $|\psi_i|^2 > \epsilon$, can then be defined to select bound or unbound states to compute transitions. This metric, however, is not always successful in separating quasi-bound states, such as those which predissociate

¹github.com/Exomol

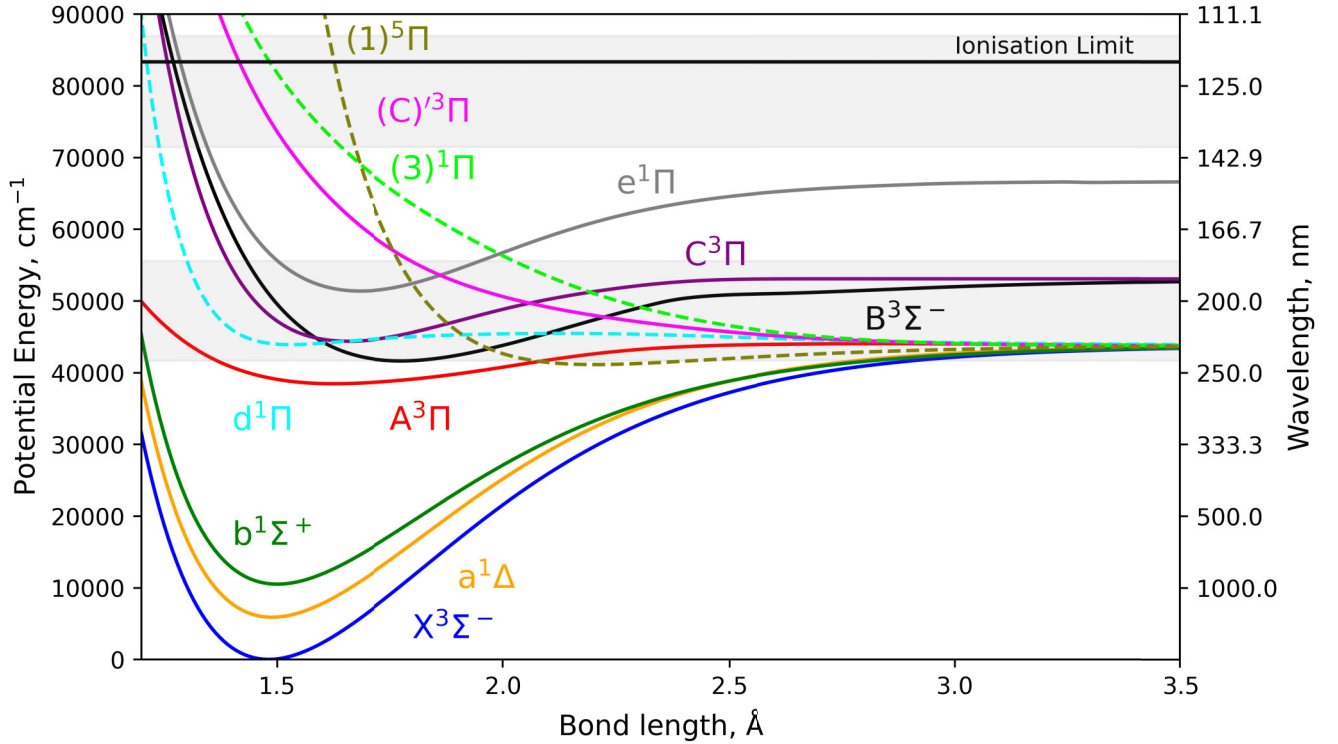


Figure 1. PECs of the electronic states considered in this work. The solid lines are states included in the final transition calculations, and the dashed lines indicate additional states included in stabilization calculations for predissociation line widths. The shaded regions mark the spectroscopic regions covered by the room-temperature experimental cross-sections presented in the Leiden data base.

(see Section 2.6), since they have an oscillating wavefunction towards large stretches yet remain highly localized at the potential minimum (A. Sokolov et al. 2025). A second metric is then employed, which compares the bond length expectation value of the wavefunction $\langle r \rangle$ (A. G. Császár et al. 2020). Unbound wavefunctions will have $\langle r \rangle$ which sits near the middle of the bond length grid considered, whereas (quasi-)bound states will typically have shorter average bond lengths centred nearer the potential minimum.

With this, we define a state as unbound and contributing to bound-free photoabsorption by having an expectation value of $\langle r \rangle > 3.55$ Å. All other states then enter the bound-bound transition calculations, where we consider predissociative effects. Further post-processing for different electronic states was required to provide more refined separation of bound-unbound states. A detailed discussion on this method is provided by A. Sokolov et al. (2025).

2.3 MARVEL: empirical energies

A self-consistent set of rovibronic energy levels is made through a weighted linear least squares procedure via inversion of experimental transition data using the MARVEL (measured active rotational vibrational energy levels) procedure (T. Furtenbacher, A. G. Császár & J. Tennyson 2007; T. Furtenbacher & A. G. Császár 2012a). The MARVEL algorithm is built using elements of network theory in production of a spectroscopic network (SN) (A. G. Császár & T. Furtenbacher 2011; T. Furtenbacher & A. G. Császár 2012b). Inversion of the transition data then yields not

only a set of associated energy levels, but also their uncertainties. An iterative re-weighted protocol then achieves self consistency within the energy levels by adjusting the uncertainties in the line positions. An optimized uncertainty σ_{opt} is then retrieved, such that each energy level until agrees with the rest of the network.

In this study, we use the MARVEL data set for SO presented by R. P. Brady et al. (2023), who provide a comprehensive description on the data sources analysed. Particularly, the $B^3\Sigma^-$ and $C^3\Pi$ energies from this network are used to refine our spectroscopic model, and is discussed in Section 2.5.

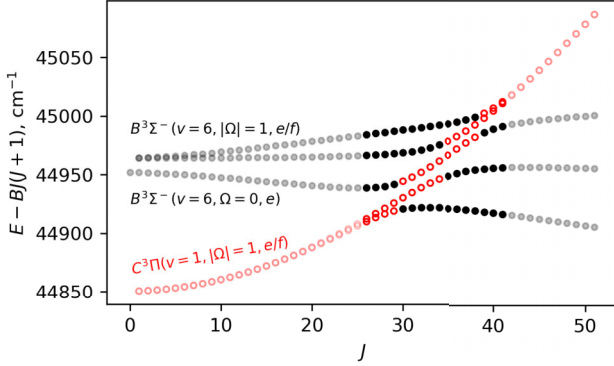
2.4 Spectroscopic models

The spectroscopic model we employ for studying the photodissociation of SO is largely based off of the SOLIS line list model (R. P. Brady et al. 2023), with the addition of the $C^3\Pi$, $C'^3\Pi$, $d^1\Pi$, $(3)^1\Pi$, and $(1)^5\Pi$ states. We chose to exclude the $A'^3\Delta$ and $A''^3\Sigma^+$ from our spectroscopic model since their spectrum does not enter the photodissociation cross-sections and we observed that their coupling to the predissociative states contributed negligible line width. C.-P. Liu et al. (2006) suggests that the $B^3\Sigma^-$ is perturbed by $A''^3\Sigma^+$, but its inclusion revealed it contributed negligible predissociation in the $B^3\Sigma^-$ state. Therefore, to reduce computational cost of running nuclear motion calculations, they were excluded.

Table 1 summarizes the states included in our spectroscopic model at different stages of our calculations. The details of these choices are then made in the subsections below.

Table 1. Summary of the electronic states included in our spectroscopic model at different stages of our nuclear motion calculations.

Calculation	$X^3\Sigma^-$	$a^1\Delta$	$b^1\Sigma^+$	$A^3\Pi$	$B^3\Sigma^-$	$C^3\Pi$	$d^1\Pi$	$e^1\Pi$	$(3)^1\Pi$	$C'^3\Pi$	$(1)^5\Pi$
Refining	✓	✓	✓	✓	✓	✓				✓	
Stabilization	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Line list	✓	✓	✓	✓	✓	✓		✓		✓	

**Figure 2.** Reduced term plot of the rotational progression of the SO MARVEL $B^3\Sigma^-(v=6)$ (closed circles) and $C^3\Pi(v=1)$ (open circles) energies using a rotational constant of $B = 0.47 \text{ cm}^{-1}$. The high opacity region serves to highlight the resonance between these states (see text). This demonstrates the excellent assignment by A. N. Heays et al. (2022) and the complicated task of fitting our model to these resonances.

2.5 Refinement to MARVEL energies

The coupling mechanisms driving the predissociation of the $B^3\Sigma^-$ and $C^3\Pi$ states of SO are inherently complex, making the refinement of the SO model against experimental data a challenge for multiple reasons. Three primary obstacles were identified:

Non-adiabatic and resonance effects: As discussed in previous work (C.-P. Liu et al. 2006; A. N. Heays et al. 2022; R. P. Brady et al. 2023), the rovibrational levels of the $B^3\Sigma^-$ and $C^3\Pi$ states exhibit numerous resonances and complex avoided-crossing structures with the unresolved $(3)^3\Sigma^-$ (K. Sarka & S. Nanbu 2019) and $C'^3\Pi$ states, respectively. Fig. 2 is a reduced term plot illustrating a resonance between the $B^3\Sigma^-(v=6)$ and $C^3\Pi(v=1)$ states. Within this localized region, the $B^3\Sigma^-$ sublevels increase in energy in the order of $(\Omega=0, e)$, $(\Omega=1, f)$, and $(\Omega=1, e)$. Similarly, the $C^3\Pi$ sublevels follow an energy ordering of $(|\Omega=1|, e)$ followed by $(|\Omega=1|, f)$. These resonances and the non-adiabatic couplings made an initial fit to empirical MARVEL (measured active rotation-vibration energy levels) data (R. P. Brady et al. 2023) computationally intractable at the time of publishing our SOLIS line list.

Extended state coupling: Subsequent analysis in this study identified that coupling to the $(1)^5\Pi$, $d^1\Pi$, and $(3)^1\Pi$ states significantly contributes to the predissociation of $B^3\Sigma^-$ and $C^3\Pi$, further complicating nuclear motion calculations.

Predissociation broadening: Heavy predissociation in the $B^3\Sigma^-$ and $C^3\Pi$ spectra (E. V. Martin 1932; C.-P. Liu et al. 2006; L. Yu & W. Bian 2011; A. N. Heays et al. 2022) results in broadening on the order of 10^0 – 10^1 cm^{-1} . Furthermore, our solution to the time-independent diatomic Schrödinger equation discretises continuum states within a finite ‘box’ of bond length grid points.

Without a computationally expensive stabilization procedure at every iteration (which remains prohibitive) the rovibronic levels can deviate from their stabilized values by up to several predissociation widths of the given level. It was seen that the many $B^3\Sigma^-$ states were not stable, and so the accuracy of the fit is limited. For a detailed discussion on this see Section 2.5.1.

Despite these limitations, recent advances in treating non-adiabatic couplings, diabaticization, and numerical techniques within the DUO nuclear motion code (S. N. Yurchenko et al. 2016) have made fitting these states feasible. While a global fit including all states (including $A'^3\Delta$ and $A''^3\Sigma^+$) proved impossible to maintain consistent quantum number labelling amidst the forest of states, a pragmatic reduced model approach was adopted.

To produce photodissociation rates, which do not necessitate high-resolution spectroscopic accuracy, the $B^3\Sigma^-$ and $C^3\Pi$ were fitted to MARVEL energy levels using a reduced model consisting of the $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, $B^3\Sigma^-$, $C^3\Pi$, and $C'^3\Pi$ states. Here, we utilize the $B^3\Sigma^-$ and $C^3\Pi$ MARVEL energies presented and discussed by R. P. Brady et al. (2023) to refine our current spectroscopic model. The line positions were later empirically corrected through a MARVELization procedure (see Section 3.1). The refinement of the intensities, where predissociative effects are fully encountered, are discussed in Section 3.3.

Refining the $B^3\Sigma^-$ PEC was tricky due to the shoulder appearing at $v=15$ because of an avoided crossing with the unresolved $(3)^3\Sigma^-$ state. Many attempts in modelling this potential by diagonalising a two-state diabatic model (for method details see examples by R. P. Brady et al. 2024, R. P. Brady 2025, R. P. Brady & S. N. Yurchenko 2025, S. N. Yurchenko et al. 2024) produced energies which were well modelled near the avoided crossing, but was difficult to constrain near minimum and dissociation. This can be attributed to the diabatic potential minimum shifting in energy relative to the adiabatic one, and is the parameter we use in fitting which is unfortunately not well constraining of the states near minimum. Additionally, R. P. Brady (2025) discuss how non-zero diabatic coupling near the minimum necessitate larger contracted vibronic basis sets for convergence, which increased computational time. Instead, we took the numerical grid-based potential fitted by A. N. Heays et al. (2022), and then morphed this curve to a Šurkus-like expansion (L. Prajapat et al. 2017; S. N. Yurchenko et al. 2018a) given by

$$F(r) = \sum_{i=0}^N B_i z^i(r)(r - \xi_p) + \xi_p B_\infty, \quad (1)$$

where B_i are the expansion coefficients, B_∞ is usually taken as zero in-order to prevent the expansion from diverging towards $r \rightarrow \infty$, $\xi_p(r)$ is the so called Šurkus variable (A. A. Šurkus, R. J. Rakauskas & A. B. Bolotin 1984) given by

$$\xi_p(r) = \frac{r^p - r_e^p}{r^p + r_e^p} \quad (2)$$

with p as an integer parameter to allow for a better convergence at large bond lengths values and effectively controls the ‘variability’/‘responsiveness’ of the polynomial with r . Finally, z is a damped displacement coordinate given by

$$z(r) = (r - r_e) \exp[-\beta_2(r - r_e)^2 - \beta_4(r - r_e)^4], \quad (3)$$

where β_2 and β_4 are damping constants which prevent large oscillations of the function asymptotes which are not well constrained by the data. Furthermore, SOCs and EAMCs were also fitted by morphing the *ab initio* data points using equation (1). The $B^3\Sigma^-$ state was then fitted by floating the expansion parameters of equation (1).

To fit $C^3\Pi$, we transformed our spectroscopic model into the diabatic representation for the Hilbert space containing $C^3\Pi$ (i.e. PECs and all couplings involving the $C^3\Pi$ and $C'^3\Pi$). This diabaticization was initially done to the *ab initio* spectroscopic model by R. P. Brady et al. (2022), and is adopted here. We then represent the diabatic $C^3\Pi$ using an Extended Morse Oscillator (EMO) function, given by

$$V(r) = V_e + D_e \left(1 - \exp \left[- \left(\sum_{i=0}^N a_i \xi_p(r)^i \right) (r - r_e) \right] \right)^2, \quad (4)$$

where D_e is the dissociation energy, V_e is the potential minimum, a_i are the expansion coefficients, r_e is the equilibrium bond length, and $\xi_p(r)$ is given by equation (2). The unbound $C'^3\Pi$ is left *ab initio* on a grid of points and is interpolated using (natural) cubic splines on to our computation grid. The diabatic coupling between the $C^3\Pi$ and $C'^3\Pi$ is also left on a grid of points and is computed from the diabaticization of the *ab initio* PECs by R. P. Brady et al. (2022). The diabatic $C^3\Pi$ was then fitted by floating the parameters of the EMO function.

We fit 99.8 per cent of the $B^3\Sigma^-$ energy levels with a weighted root mean square error (wRMSE) of 5.65 cm^{-1} and 95.3 per cent of the $C^3\Pi$ energy levels with a wRMSE of 3.45 cm^{-1} . The remaining states were identified as misassigned by quantum numbers by our code, and we exclude them from the wRMSE calculation. The weights used in the wRMSE calculation are defined in equation (5) of R. P. Brady et al. (2023). Fig. 3 illustrates the absolute residuals of our computed energy levels for these states relative to the empirical MARVEL energies.

While our model does not reproduce all empirical MARVEL energies to high-resolution spectroscopic accuracy (with some highly excited vibrational states deviating by tens of wavenumbers), the reason for these discrepancies is threefold: (1) we do not account for couplings to additional excited electronic states crossing the $B^3\Sigma^-$ potential, as investigated by L. Yu & W. Bian (2011), C.-P. Liu et al. (2006); (2) the absence of experimental transition data to the $B^3\Sigma^-$ ($v=0$) state prevents the extraction of its ground rovibronic energy from the MARVEL network, leaving the potential minimum poorly constrained and introducing degeneracy into the fit; and (3) the strong perturbation between the $B^3\Sigma^-$ and $C^3\Pi$ means their computed energy terms are highly correlated, limiting independent refinement (as detailed in Section 2.5.1).

Lower lying vibrational states are generally better reproduced by our model, as the dominant interactions in this region are mostly between $B^3\Sigma^-$ and $C^3\Pi$. While couplings to $d^1\Pi$, $A''^3\Sigma^+$, and $A'^3\Delta$ states do slightly perturb these lower vibrational levels, we find their influence to be negligible compared to the primary $B^3\Sigma^-$ – $C^3\Pi$ interaction. More importantly, attempting to include these minor couplings at the current level

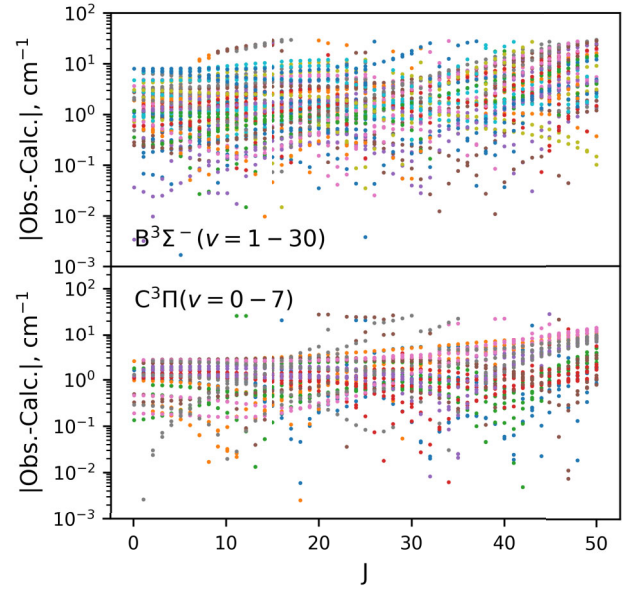


Figure 3. Observed (empirical MARVEL) minus calculated energies as a function of the rotational quantum number J for the $B^3\Sigma^-$ and $C^3\Pi$ states. Different colours indicate the vibrational quantum number v .

of model accuracy yields negligible improvements in the energy terms while introducing widespread quantum number misassignments. These misassignments severely impact the accuracy of assigning correct predissociation lifetimes, detailed in Section 4.2. Consequently, these states were excluded in favour of a more stable, reduced model.

As demonstrated in Sections 2.6 and 3.3, this reduced model accurately reproduces experimental radiative and predissociation lifetimes, ensuring our calculated transition intensities remain robust despite the exclusion of these weaker couplings. Furthermore, the energy residuals seen here, even if the states were left un-MARVELized, would have a negligible impact on our final computed photorates (see Section 4.2 for details). Shifting the entire spectrum by $+20 \text{ cm}^{-1}$ results in a fractional change in the photorates of less than 1 per cent in the worst case (for cooler radiation temperatures). This extreme test case highlights that transitions to the few rovibronic states with residuals on the order of 10 cm^{-1} will have a negligible impact on the associated photodissociation rates, since a fraction of the intensity will be shifted across a wavelength region where the stellar flux is effectively constant.

Finally, because our empirical MARVEL data set covers nearly the entire potential well of both the $B^3\Sigma^-$ and $C^3\Pi$, our subsequent MARVELization procedure replaces these computed energies with empirical data, correcting nearly all relevant line positions to experimental accuracy prior to cross-section generation. Therefore, our model robustly captures the underlying physics required for obtaining accurate photodissociation rates.

2.5.1 Accuracy limiting predissociation widths

Since we rely on a stabilization methodology to retrieve the predissociation broadening half widths and line centres from our spectroscopic model (see Section 2.6), when fitting our model to experimental data we are forced to choose an arbitrary box size for energy level calculations (S. N. Yurchenko et al. 2016).

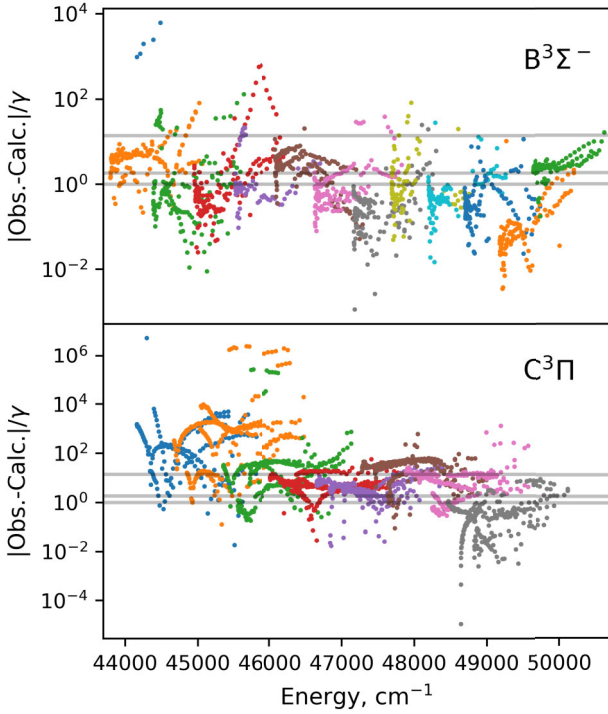


Figure 4. Computed predissociation width weighted residuals for the $B^3\Sigma^-$ and $C^3\Pi$ states as a function of energy, where horizontal lines indicate 1Γ , 1.84Γ , and 13.9Γ thresholds. Different colours indicate different vibrational states.

Consequently, each calculated state energy represents a random sample from a Cauchy distribution governed by the state’s underlying predissociative coupling. While the ideal fitting procedure would target the stabilized resonance centres (E_0), performing a full stabilization at every iteration is computationally intractable.

Therefore, the accuracy of our spectroscopic model is fundamentally bounded by the intrinsic width of each state. Attempting to refine the PECs or coupling terms to match experiment significantly better than the associated half width is physically uninformative. Consequently, ‘over-fitting’ would likely introduce unphysical features to the PECs and couplings merely to account for sampling noise. To assess the model’s performance rigorously, energy residuals must be evaluated relative to each state’s predissociation width, as even an exact physical model would exhibit residual variance on the order of the predissociation broadening within our framework. Fig. 4 illustrates the width normalized residual for the $B^3\Sigma^-$ and $C^3\Pi$ rovibronic levels, defined by

$$\mathcal{R} = \frac{|E_{\text{MARVEL}} - E_{\text{Calculated}}|}{\Gamma}, \quad (5)$$

where Γ is the predissociative half width. The horizontal lines (in ascending order) represent the 50 per cent (HWHM), 68 per cent (1σ equivalent), and 95 per cent (2σ equivalent) percentiles, marking the probability of randomly sampling an energy level within 1Γ , 1.84Γ , and 13.9Γ (computed by inverting the Cauchy cumulative distribution function) of the resonance centre. We see that the majority of $B^3\Sigma^-$ levels sit within 1Γ , with a median $\mathcal{R}$ of 0.8. This suggests we have fit the $B^3\Sigma^-$ spectroscopic model as much as possible, and even slightly over-fitted some states. The $C^3\Pi$ state, however, has a median $\mathcal{R}$ of 8.9, where the

Table 2. Comparison of the median width normalized residual ($\mathcal{R}$) and wRMSE of the fitted $B^3\Sigma^-$ and $C^3\Pi$ energy levels.

State	Median $\mathcal{R}$	wRMSE (cm^{-1})
$B^3\Sigma^-$	0.81	5.65
$C^3\Pi$	8.92	3.45

majority of levels sit outside the the 1Γ region about the energy centre. This can be understood since the widths for the $C^3\Pi$ are much narrower than for $B^3\Sigma^-$, despite the wRMSE being lower than for $B^3\Sigma^-$. As detailed in Table 2, both $\mathcal{R}$ and the wRMSE for the fitted $B^3\Sigma^-$ and $C^3\Pi$ energies summarise these metrics. This suggests the model can be improved further, however with the caveat that $B^3\Sigma^-$ and $C^3\Pi$ are strongly coupled and their PECs strongly overlapping. The accuracy of our $C^3\Pi$ energies are then dependent on the accuracy of $B^3\Sigma^-$, for example to correctly reproduce the rovibronic resonances. Since we cannot statistically improve the computed $B^3\Sigma^-$ energies without risk of over-fitting, we conclude our spectroscopic model is as accurate as possible without further method development. Regardless, we MARVELize our final computed line list to correct for the line positions, and is discussed in Section 3.1.

2.6 Predissociation broadening

Transitions to predissociative states appear diffuse but retain structure similar to bound–bound transitions. This diffuseness arises from the quasi-bound nature of states above the dissociation limit which exhibit unbound character through mechanisms described by G. Herzberg (1939). We focus on Type I predissociation, where rovibronic states couple to the continuum arising from a nearby dissociative electronic state. The width of broadening, or equivalently the reduction in state lifetime, depends on the coupling strength and the overlap of the respective wavefunctions (U. Fano 1961). Consequently, crossings with dissociative states induce strong local predissociation.

Fig. 5 illustrates the complex curve crossings with the $B^3\Sigma^-$ and $C^3\Pi$ states, involving PECs of strong non-adiabatic character and curve crossing at both inner and outer limbs of the PECs. Previous studies (L. Yu & W. Bian 2011; A. N. Heays et al. 2022) identified the $(1)^5\Sigma^-$, $d^1\Pi$ (weak), $A^3\Pi$, $C^3\Pi$, $C'^3\Pi$, and $(3)^1\Pi$ states as the primary drivers of predissociation for $B^3\Sigma^-$ ($v \leq 14$). Because our original SO models (R. P. Brady et al. 2022, 2023) omitted the quintet state, we have supplemented our model with a Morse-oscillator PEC derived from *ab initio* spectroscopic constants and digitized SOCs presented by L. Yu & W. Bian (2011). For $B^3\Sigma^-$ ($v > 14$), additional crossings with unbound states exist (C.-P. Liu et al. 2006; L. Yu & W. Bian 2011), but corresponding PEC data are unavailable. However, predissociation broadening is expected to peak at $v = 14$ and 17 (R. Colin 1969; M. A. A. Clyne & P. H. Tennyson 1986; A. N. Heays et al. 2022) for the $B^3\Sigma^-$ state; transitions to energetically higher states will then be situated outside the ground state Franck–Condon (FC) region and also exhibit electronic character exchange due to avoided crossings where the vibrational transition moments drop. Consequently, for $v > 14$, we assume 100 per cent predissociation efficiency and omit these additional electronic states to focus on the most intense regions of the $B^3\Sigma^-$ – $X^3\Sigma^-$ band.

We then define our full spectroscopic model to include predissociative coupling, where the included electronic states are summarized in Table 1. The final state lifetime for the quasi-

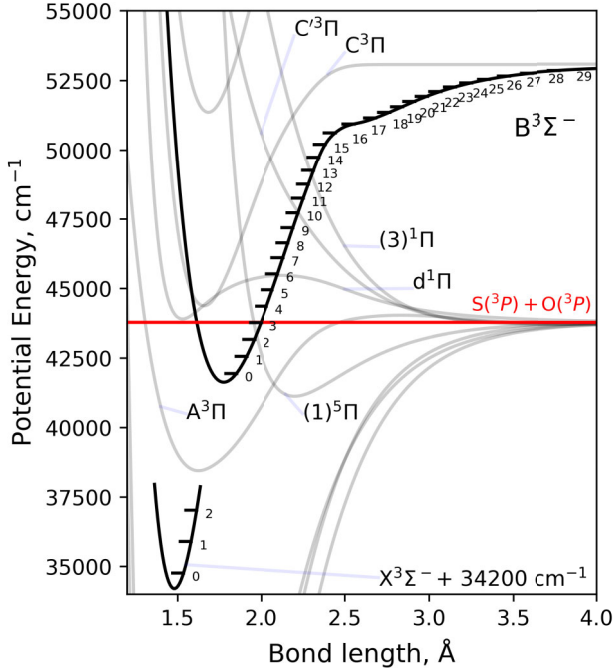


Figure 5. State crossings with $B^3\Sigma^-$ (bold) and its corresponding vibrational energies superimposed on the PEC. The horizontal line indicates the dissociation asymptote to which we focus our treatment on. The solid PEC in the bottom left is a section of the $X^3\Sigma^-$ potential shifted +34200 cm^{-1} to indicate the horizontal shift of the ground state relative to $B^3\Sigma^-$.

bound states are a combination of the radiative lifetime, τ_{rad} , and the predissociation lifetime, τ_{pred} , according to the following summation of the corresponding rates k

$$k_{\text{total}} = k_{\text{rad}} + k_{\text{pred}} = \frac{1}{\tau_{\text{rad}}} + \frac{1}{\tau_{\text{pred}}}, \quad (6)$$

where the final state lifetime is given by

$$\tau_{\text{total}} = \frac{1}{k_{\text{total}}}. \quad (7)$$

The radiative lifetime comes as a direct solution from our DUO calculations, however to compute the predissociative lifetime we adopt a stabilization procedure (A. U. Hazi & H. S. Taylor 1970; V. A. Mandelshtam, T. R. Ravuri & H. S. Taylor 1993; G. B. Mitev et al. 2025). Stabilization works by repeating energy calculations for different simulation box sizes (L_{max}), where the discretized continuum will drop in energy. As the continuum rovibronic states pass through a quasi-bound state, the resulting coupling induces an energy shift in the level. The broadening half width, Γ , is extracted by fitting the energy distribution of the shifting quasi-bound state to a Lorentzian profile. Fig. 6 illustrates an example stabilization plot for a quasi-bound state. The predissociation lifetime is then computed from Γ via

$$\tau_{\text{pred}} = \frac{1}{4\pi c\Gamma}, \quad (8)$$

where c is the speed of light in cm s^{-1} .

In order to determine the fraction of the total computed SO cross-section which leads to photodissociation via predissociation, we need to scale the Einstein A coefficients in the .TRANS

file by the so called predissociation efficiency η defined by

$$\eta = \frac{k_{\text{pred}}}{k_{\text{total}}}. \quad (9)$$

The scaled Einstein A coefficient for a transition from some bound state ‘ i ’ to a quasi-bound state ‘ f ’ is then

$$\tilde{A}_{fi} = \eta_f A_{fi}. \quad (10)$$

Thus, when considering transitions between two truly bound states, $\eta = 0$ and $\tau_{\text{pred}} = 0.0$, whereas $\eta = 1$ would mean the upper state leads to the fragmentation of the diatomic without chance to radiatively decay to some lower state. Fig. 7 illustrates the computed predissociation efficiencies for the $B^3\Sigma^-$ and $C^3\Pi$ rovibronic levels. We see that all states above the first dissociation limit are nearly 100 per cent predissociative, and so we expect that transitions to these states will entirely contribute to photodissociation of SO and will thus be important for the photodissociation rate. A small subset of $B^3\Sigma^-$ rovibronic states exhibit reduced predissociation efficiencies of 30–80 per cent, corresponding to instances where the total energy is pushed just above the dissociation limit by rotational excitation, despite the underlying vibrational level lying below the continuum. With this, to extrapolate our treatment of higher lying rovibronic states of $B^3\Sigma^-$, which our model does not include the necessary electronic states to encounter the full predissociative continuum coupling, we assume 100 per cent predissociation efficiency when computing the final cross-sections, and set the widths via extrapolating our fitted widths as functions of J and Ω , and take the experimental values where possible (see discussion below). Therefore, by scaling the Einstein coefficient by η , we properly recover the predissociative contribution to the photodissociation cross-section. We then modify the lifetime in the .STATES file by replacing the radiative one with the total lifetime from equation (7), which is subsequently used to calculate line broadening when computing cross-sections.

A. N. Heays et al. (2022) provide a comprehensive analysis of $B^3\Sigma^-$ and $C^3\Pi$ predissociation, with predissociative half-widths fitted to recorded spectra as functions of v and Ω . It is not explicitly stated whether these parameters represent $J = 0$ values, rotationally averaged widths, or values derived from specific $J > 0$ transitions. Fig. 8 compares our computed predissociation lifetimes (for multiple J) to the experimental values of A. N. Heays et al. (2022). We observe agreement for both the $B^3\Sigma^-$ and $C^3\Pi$ states within experimental uncertainty. For $B^3\Sigma^-(v > 15)$, where our theoretical model is truncated due to unavailable electronic state data (see discussion above), we adopt the experimental lifetimes for all J . Notably, we provide predicted lifetimes for $C^3\Pi(v = 0)$, for which experimental data is absent. A visible discrepancy occurs at $B^3\Sigma^-(v = 8)$, where the experimental lifetimes exhibit a localized increase that is less pronounced in our calculations. This is consistent, however, with the curve crossing topology in Fig. 5, where $B^3\Sigma^-(v = 8)$ is situated in a region of lower state density. Given the absence of reported uncertainties for these experimental points, and the fact that our results follow a smoother trend consistent with neighbouring vibrational levels, we argue that our model provides a physically consistent representation of the broadening. Finally, the shorter experimental lifetimes observed for $B^3\Sigma^-(v = 14, 15, \Omega = 0)$ likely reflect the influence of additional electronic curves and couplings in this high-energy region not currently included in our Hamiltonian.

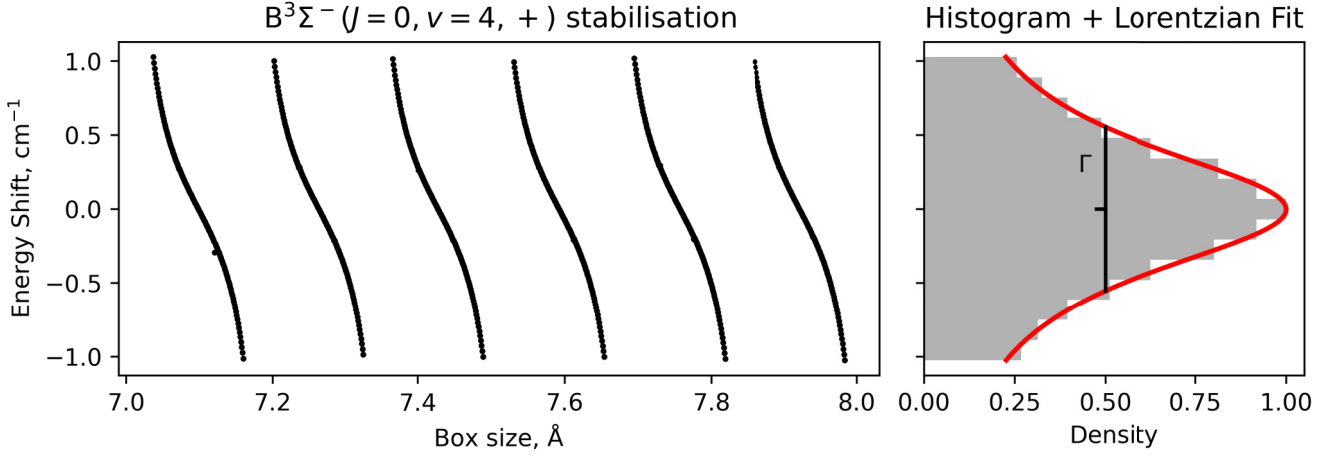


Figure 6. Stabilization of a rovibronic energy level as the simulation box size increases, a series of resonances occur (left panel). The predissociation broadening width Γ is then obtained by fitting a Lorentzian function to the energy distribution about its stable point (right panel), the centroid (shifted to 0 here).

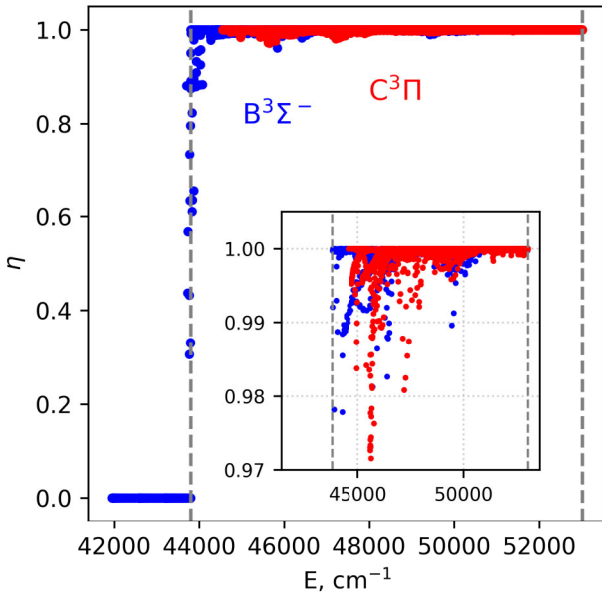


Figure 7. Computed predissociation efficiencies of the B³Σ⁻ and C³Π state levels. Some structure is seen in the efficiencies, however, nearly all states above the first dissociation limit (leftmost vertical line) are practically 100 per cent predissociative.

3 LINE LIST

Towards calculating SO photodissociation rates, we require two components of the SO cross-section; predissociated bound-quasi-bound transitions and direct continuum photoabsorption through bound-free transitions. We compute both line lists through input of the spectroscopic model outlined in the ‘Line List’ row of Table 1 input to the DUO programme. For the nuclear motion calculations, a vibrational sinc-DVR basis of (58, 58, 58, 58, 350, 350, 350, 350) functions for the X³Σ⁻, a¹Δ, b¹Σ⁺, A³Π, B³Σ⁻, C³Π, e¹Π, and C³Π was used, respectively. In all calculations, we compute states up to $J = 200$, where the partition

function (PF) is converged for all temperatures considered here (see Section 3.2).

3.1 Line list MARVELization

To enhance the accuracy of our computed line positions, energy levels in the .states files (and consequently transition frequencies in the .trans files) are replaced by empirically determined values from the MARVEL SN (R. P. Brady et al. 2023) through a process known as ‘MARVELization’ (L. K. McKemmish et al. 2024). While this improves transition frequencies for states within the network, it does not extend the predictive power of the line list beyond that coverage. Following the approach of L. K. McKemmish et al. (2024), we implemented the predictive shift method (C. A. Bowesman et al. 2021) for the X³Σ⁻, a¹Δ, b¹Σ⁺, and A³Π levels. This method fits the ‘Observed minus Calculated’ (Obs.-Calc.) trends as a function of J for each vibrational and Ω trajectory, allowing for the interpolation of gaps or extrapolation to higher J values. For the B³Σ⁻ and C³Π levels, however, we opted for simple MARVELization rather than predictive shifts; our tests indicated that misassigned levels in these states caused the predictive shifts to erroneously interpolate toward different electronic states.

We also propose a complementary method to improve line list accuracy by incorporating energy terms from highly tuned spectroscopic models. The introduction of additional electronic states and the refinement of PECs and couplings to the B³Σ⁻ and C³Π states led to minor shifts in the X³Σ⁻, a¹Δ, b¹Σ⁺, and A³Π levels, which slightly worsened the fit to MARVEL data. To resolve this, we replaced all non-MARVEL energy terms for these states with values from our previous high-resolution SOLIS line list (R. P. Brady et al. 2023). Similarly, the B³Σ⁻ and C³Π levels not covered by MARVEL were replaced with values from the refined model described in Section 2.5. By combining these methods, we achieve the highest possible accuracy across all electronic states considered in this study.

A new set of calculated energy source labels is then introduced and are summarized as follows: ‘C0’ are calculated energies from the line list spectroscopic model; ‘C1’ are calculated energies from

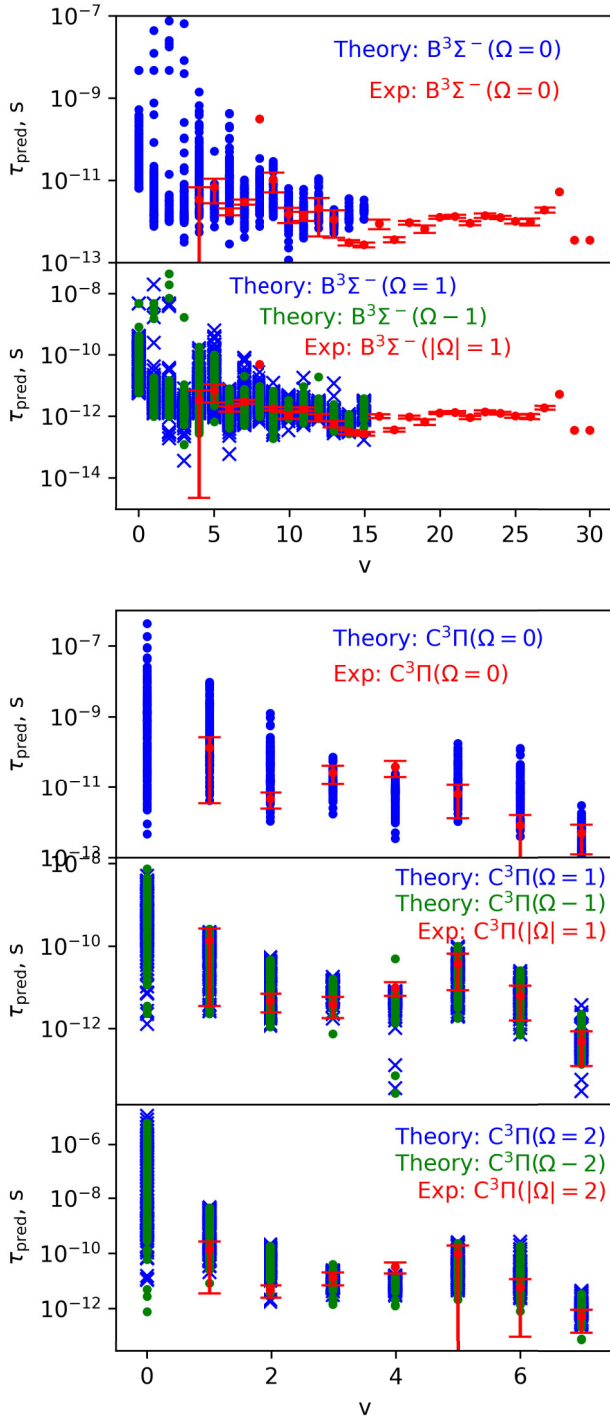


Figure 8. Comparison of computed predissociation lifetimes (all J) with experimental values from A. N. Heays et al. (2022) for the $B^3\Sigma^-$ ($\Omega = 0, \pm 1$) and $C^3\Pi$ ($\Omega = 0, \pm 1, \pm 2$) states.

the SOLIS line list (R. P. Brady et al. 2023); ‘C2’ are calculated $B^3\Sigma^-$ and $C^3\Pi$ energies from the fitted spectroscopic model.

This hybrid line list then presents an update to our previous SOLIS line list (R. P. Brady et al. 2023), where we extend the accurate treatment to the $B^3\Sigma^-$ and $C^3\Pi$ states. This updated line list, SOLUVIS, then spectroscopically covers wavelengths longer than 120 nm ($< 83333.33 \text{ cm}^{-1}$) and is available in the Ex-

oMol data base (<https://www.exomol.com/>) in the form of States (.states) and Transition (.trans) files.

3.2 Partition function

The SO PF computed from our line list is nearly identical to our previous results (R. P. Brady et al. 2023) and aligns well with values from A. J. Sauval & J. B. Tatum (1984), P. S. Barklem & R. Collet (2016), and CDMS (C. P. Endres et al. 2016).

As shown in Fig. 9, assuming LTE, SO is almost exclusively populated in its $X^3\Sigma^-$ ground electronic state at temperatures up to 5000 K. While the $a^1\Delta$ state population only reaches 1 per cent at 5000 K, transitions from this state may still contribute to the spectra of extremely hot astrophysical objects (R. P. Brady et al. 2022). Fig. 10 demonstrates that our chosen $J_{\text{max}} = 200$ ensures PF convergence across the entire temperature range studied.

Fig. 10 displays the convergence of the SO PF with the rotational quantum number J at various temperatures. We determined the minimum J_{max} values required for the PF to reach 90 per cent, 95 per cent, and 99 per cent of its total value. We find that the maximum J value of 200 used in our line list is sufficient to converge the PF across all temperatures considered. Furthermore, our MARVEL energies cover up to $J \sim 50$, providing convergence for temperatures between approximately 750 and 1250 K. For objects cooler than these thresholds, the line positions provided for $J \leq 50$ should achieve experimental accuracy.

3.3 Radiative lifetimes and scaling DMCs

Electric dipole moments, lifetimes, and direct intensity measurements can be used to constrain our *ab initio* DMCs. R. P. Brady et al. (2023) discuss how specific dipoles were constrained in the SO spectroscopic model, which we extend in this work. For the UV region, A. N. Heays et al. (2022), J. M. F. Elks & C. M. Western (1999), and K. Yamasaki et al. (2005) report rotationless radiative lifetimes for the $B^3\Sigma^-$ ($v = 0, 1, 2, 3$) states which we use to constrain our *ab initio* $\langle X^3\Sigma^- | \mu_z | B^3\Sigma^- \rangle$ TDMC (R. P. Brady et al. 2022). R. P. Brady et al. (2023) formulated an approximate scaling relation between lifetime and dipole moment (their equation 15), showing that a scaling in lifetime $\tilde{\tau} = \xi \tau$ corresponds to an approximate scaling in the dipole moment to the dominant lower state of $1/\sqrt{\xi}$. This approximation breaks down in the presence of significant intensity borrowing through various couplings, as the scaling would only apply to one component of the transition moment. We found this to be the case for the $B^3\Sigma^-$ state, where a simple $1/\sqrt{\xi}$ scaling derived from the lifetime was insufficient. Instead, we optimized this scaling by fitting our computed radiative $B^3\Sigma^-$ ($J = 0, v = 0, 1, 2, 3$) lifetimes to the experimental (J. M. F. Elks & C. M. Western 1999; K. Yamasaki et al. 2005) and semi-empirical values (A. N. Heays et al. 2022). A scaling factor of 1.198 produced the best agreement with experimental data. Table 3 shows the radiative $B^3\Sigma^-$ lifetimes before and after optimization. While our raw *ab initio* DMC produced lifetimes approximately a factor of two larger than other sources (consistent with the conclusion drawn by R. P. Brady et al. (2022) that the $B^3\Sigma^-$ was the least accurate of their treated electronic states) our scaled results show excellent agreement with experimental and semi-empirical values. It was suggested by A. N. Heays et al. (2022) and by our work that the $B^3\Sigma^-$ ($v = 3$) radiative lifetime measured by J. M. F. Elks & C. M. Western (1999) is an anomaly; it was removed from the optimization of our dipole moment scaling.

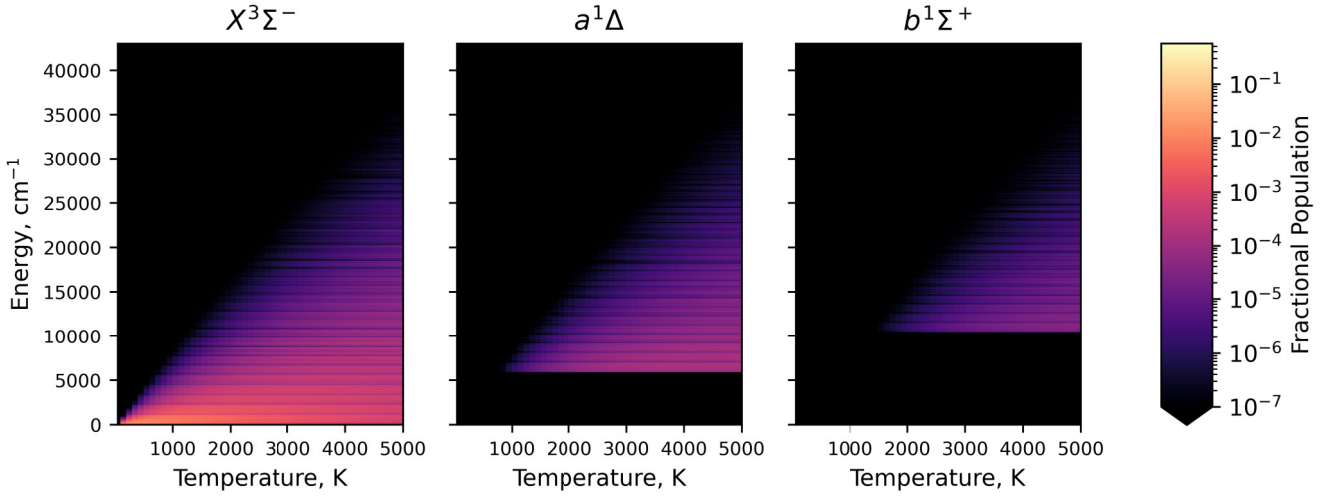


Figure 9. Fractional populations for the $X^3\Sigma^-$, $a^1\Delta$, and $b^1\Sigma^+$ states of SO as a function of temperature.

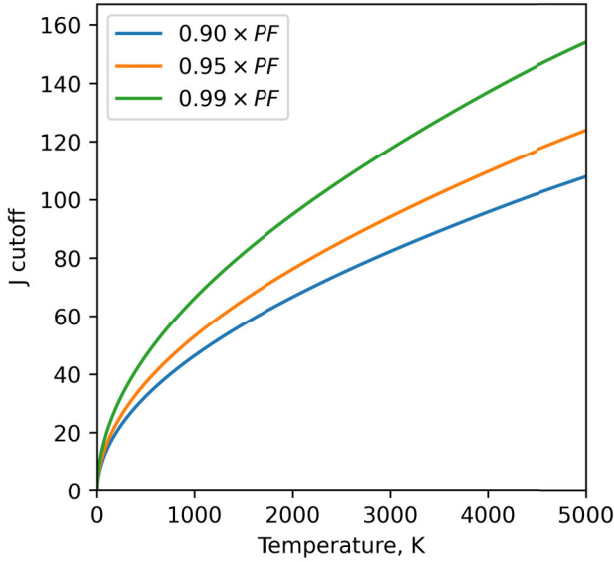


Figure 10. Convergence of the SO PF as a function of temperature and simulated maximum J .

Table 3. Radiative lifetimes (ns) for the ($J = 0$) $B^3\Sigma^-$ levels below the lowest SO dissociation limit. The data sources are indicated by: (a) A. N. Heays et al. (2022); (b) J. M. F. Elks & C. M. Western (1999); (c) K. Yamasaki et al. (2005).

v	This work	Our <i>Ab initio</i>	Semi-empirical ^(a)	Exp. ^(b)	Exp. ^(c)
0	32.1	62.1	37(4)	33.6(6)	29(2)
1	32.1	67.8	37(4)	32.3(6)	30(4)
2	32.2	77.9	38(4)	36.4(5)	27(4)
3	32.3	73.3	37(4)	52(2)	29(4)

3.4 Opacities

Temperature- and pressure-dependent opacities are precomputed as outlined by the ExoMolOP project (K. L. Chubb et al. 2021). Data are produced in four formats to support the retrieval codes ARCiS (M. Min et al. 2020), NEMESIS (P. G. J. Irwin et al.

2008), petitRADTRANS (P. Mollière et al. 2019; P. Mollière, E. Nasedkin & D. Blain 2023) and TauREx (A. F. Al-Refaie et al. 2021, 2022). The first 3 of these formats store data as correlated-k tables, while TauREx uses the photoabsorption cross-sections directly. These data all include the contribution to the overall opacity from the photodissociative processes presented in this work, in addition to the bound-bound processes previously made available. Opacities are provided over the temperature range 100–4000 K and for a pressure range of 10^{-6} – 10^2 bar, with a wavenumbers coverage of 333–50 000 cm^{-1} (30–0.2 μm).

4 PHOTODISSOCIATION CROSS-SECTIONS

Photodissociation cross-sections are computed using the EXOCROSS programme (S. N. Yurchenko, A. F. Al-Refaie & J. Tennyson 2018b) for temperatures between 1 and 10000 K, utilizing the bound-bound and bound-unbound line lists detailed in Section 3. All calculations are performed on a wavenumber grid with a resolution of 0.25 cm^{-1} , extending up to $83\,333 \text{ cm}^{-1}$ ($\geq 120 \text{ nm}$). This upper limit was chosen to safely encompass the full relevant photodissociation spectrum, noting that it slightly exceeds the experimental first ionization energy of SO (83034.2 cm^{-1} ; C.-S. Lam et al. 2011).

The computation of the bound-free line list and the resulting continuum photoabsorption cross-sections is relatively straightforward. First, discretized continuum states are separated from bound solutions using the methods described in Section 2.2, followed by the calculation of transition frequencies and Einstein A coefficients. Using this bound-free line list, EXOCROSS is used to generate the direct continuum photoabsorption cross-sections. Each discrete spectral line is broadened as a function of the vibrational quantum number using the particle-in-a-box analogy proposed by T. Uhlíková et al. (2025). This procedure yields smooth cross-sections consistent with other recent theoretical treatments of diatomic molecules (M. Pezzella et al. 2021; G. B. Mitev et al. 2025; T. Uhlíková et al. 2025; A. Sokolov et al. 2025).

The bound-quasi-bound line list and the resulting predissociation spectrum require additional processing. As detailed in Section 2.6, the contribution of bound-bound transitions to photodissociation is determined by scaling the Einstein A coefficients by the predissociation efficiency. The radiative lifetimes are then

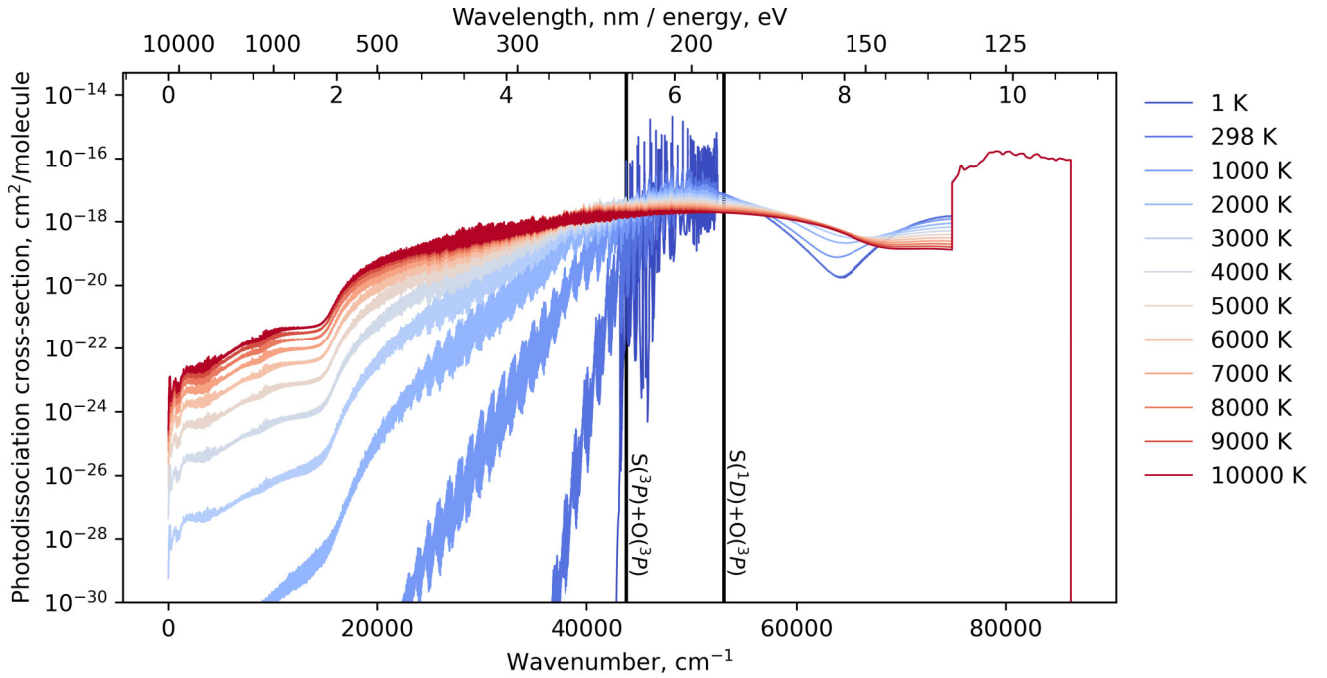


Figure 11. Our computed total photodissociation cross-sections, including predissociative bound–bound cross-sections, continuum photoabsorption cross-sections, and the Leiden top up (see text). Different colours indicate the spectrum simulated at different temperatures and the horizontal lines indicate the lowest two dissociation limits of SO.

replaced by the total lifetimes defined in equation (7). Each spectral line is broadened using a Voigt profile, where the Lorentzian component is derived from the total lifetime and the Gaussian component from the temperature. For example, the majority of the $B^3\Sigma^-$ predissociative lifetimes are on the order of a picosecond, corresponding to a HWHM of $\Gamma = 2.65 \text{ cm}^{-1}$. A wing cut-off of 100 cm^{-1} is applied to each line, with the integrated intensity beyond this threshold redistributed to the line pedestal. For the predissociation broadening considered here, this cut-off is sufficiently far from the line centres to avoid inducing discontinuities in the final spectrum.

Fig. 11 illustrates the temperature dependence of the computed total photodissociation spectrum (comprising both bound–bound and continuum photoabsorption) as a function of wavenumber, energy (eV), and wavelength (nm). At 1 K, the molecule primarily populates the ground rovibronic state. Consequently, the minimum photon energy required for photodissociation is near the lowest dissociation threshold, indicated by the solid vertical line in Fig. 11 at $\sim 43\,790 \text{ cm}^{-1}$ ($\sim 228.37 \text{ nm}$). At higher temperatures, the population of excited states increases, shifting the photodissociation threshold toward longer wavelengths. Therefore, more low-energy photons are now able to participate in molecular dissociation, leading to an increase in photodissociation rates.

Furthermore, the primary UV band of SO, $X^3\Sigma^- - B^3\Sigma^-$, exhibits a complex electronic structure that further enhances the temperature dependence of the spectrum. As shown in Fig. 5, the shift in equilibrium bond length between the $X^3\Sigma^-$ and $B^3\Sigma^-$ PECs places the FC region of the ground state near $v' = 15$ of the $B^3\Sigma^-$. This configuration has two critical implications: (1) at higher temperatures, vertical transitions from vibrationally excited $X^3\Sigma^-$ levels access lower vibrational levels in the $B^3\Sigma^-$; and (2) an avoided crossing in the $B^3\Sigma^-$ leads to an exchange in electronic character near $v' = 15$ and 16. This exchange results in

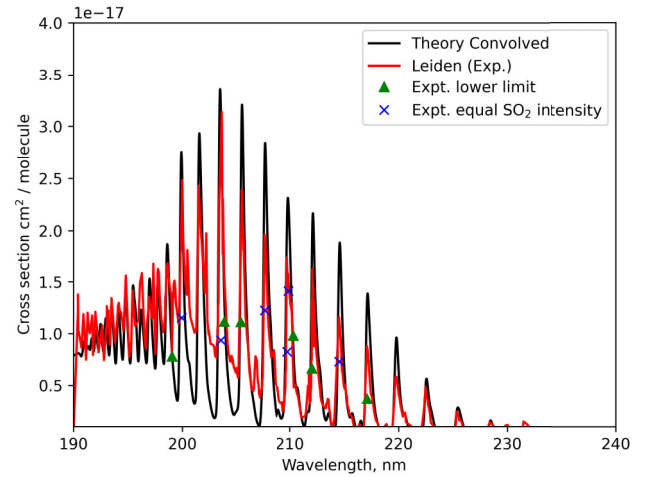


Figure 12. Comparison between our computed SO cross-sections between 190–240 nm with the experimentally recorded spectrum by L. F. Phillips (1981). Our cross-sections have been convolved with a Gaussian of 50 cm^{-1} FWHM following the comparisons made by A. N. Heays et al. (2022) to L. F. Phillips (1981). The crosses and triangles indicate regions of equal intensity by contaminating SO_2 transitions and lower experimental limits on the measured intensity, respectively.

a drastic change in the vibrational progression, a significant drop in the transition dipole moment, and a decrease in the effective rotational constant B_v (consistent with figs 12 and 15a of A. N. Heays et al. 2022 and our own calculations). Consequently, temperature variations shift the most intense transitions away from this electronic ‘turning point’, leading to a substantial change in spectral intensity. This effect is seen in Fig. 11, as well as in the

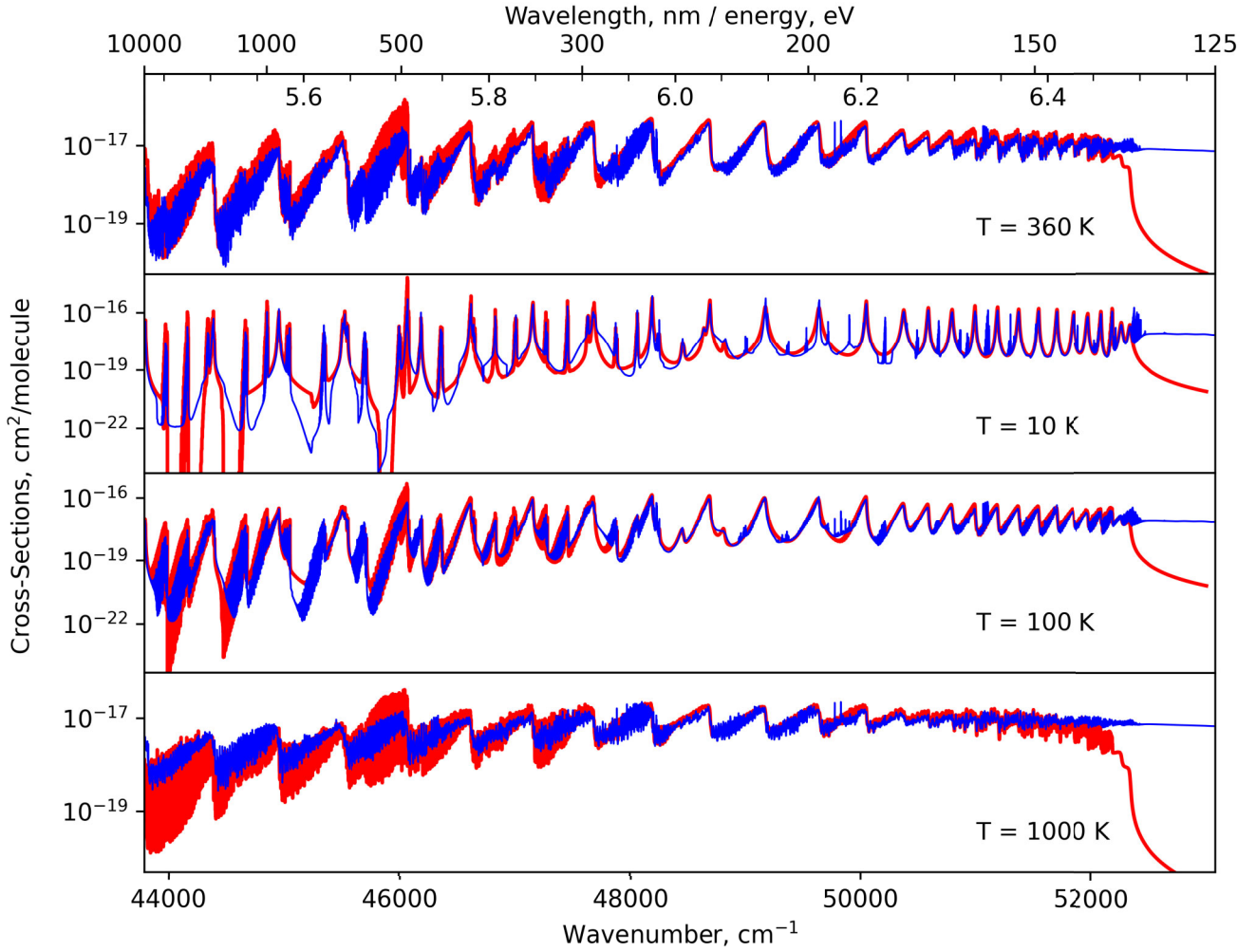


Figure 13. Comparison between our computed SO UV cross-sections (blue) to the experimental spectrum in the top panel and hybrid model spectra in the lower three panels presented by A. N. Heays et al. (2022) (red).

spectra from our previous studies (R. P. Brady et al. 2022, 2023). Combined with radiation field peaking at longer wavelengths, these molecular features result in a pronounced temperature dependence in the SO photodissociation cross-sections and rates (see Section 4.2).

Fig. 12 compares our computed photodissociation spectrum between 190 and 240 nm with the experimental measurements of L. F. Phillips (1981). To facilitate a direct comparison, our high-resolution spectrum was convolved with a Gaussian function with a 50 cm^{-1} FWHM following the same comparisons made by (A. N. Heays et al. 2022). L. F. Phillips (1981) obtained these cross-sections using a monochromator with $50 \mu\text{m}$ slits and were subsequently adopted by the Leiden data base, which estimates an uncertainty factor of 2–10 depending on the spectral region. Our results show excellent agreement with the experimental band positions, though some discrepancies in intensity persist. Specifically, as noted by (S. O. Danielache et al. 2014; A. N. Heays et al. 2022) in their comparisons to L. F. Phillips (1981), the experimental data suffer from SO_2 contamination; blue crosses denote regions where SO_2 intensity is comparable to SO, creating an underlying continuum not present in our model. Additionally, green triangles indicate the lower experimental detection limits.

While our predicted line intensities are generally higher than the measured values, they remain well within the factor of 2–10 uncertainty cited by Leiden. Given that our model incorporates high-resolution dipoles scaled to experimental lifetimes, we conclude that our line list is of high quality and accurately reproduces the experimental results.

Fig. 13 compares our computed UV ($43787.8\text{--}53074.7 \text{ cm}^{-1}$) photodissociation cross-sections with the spectra presented by A. N. Heays et al. (2022) across different temperatures. The top panel showcases the comparison with their experimental spectrum, and the lower three panels with spectrum computed using their hybrid line list. These hybrid line lists were produced by fitting spectroscopic constants, vibrational and electronic transition moments, and predissociative line widths to their experimental spectrum, band by band. We see excellent agreement in the band positions, line intensities, and band structure. One noticeable discrepancy is the spectrum towards the second dissociation limit (the high frequency cut-off of the plot), where A. N. Heays et al. (2022) spectrum decrease rapidly in intensity and become extremely smooth. Ours, however, continue at a similar intensity into the continuum where it also becomes smooth. We compared when we removed the continuum photoabsorption component of

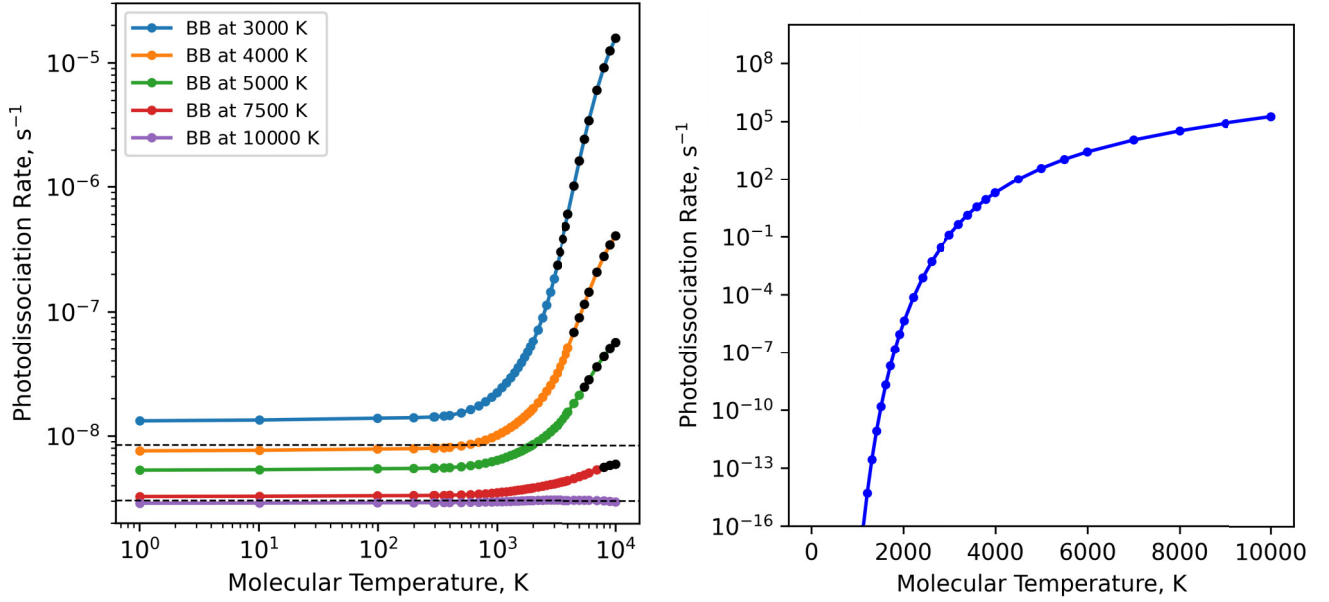


Figure 14. Fig. 14 presents SO photodissociation rates calculated via equation (11) for various blackbody radiation temperatures. Our results show good agreement with the temperature-independent Leiden rates (dashed lines). Black dots denote non-LTE conditions where the molecular temperature exceeds the radiation temperature. The right panel illustrates the strict LTE case ($T_{\text{gas}} = T_{\text{rad}}$) where the radiation field is not integral normalized to see the effect of photon number. Here, SO remains stable below 1000 K but exhibits extreme temperature dependence in the photodissociation rate above its onset at ~ 2000 K.

our cross-sections, and saw we had the same drop in intensities as theirs. Our continuum is then stronger in this region.

4.1 Short-wavelength top up

As discussed in Section 2.6, our spectroscopic model excludes the excited electronic state PECs and TDMs required to cover the UV region near the photoionization limit. This region has a negligible impact on the temperature dependence of the photodissociation rate because the radiation flux remains effectively constant over a broad range of radiation temperatures. Furthermore, the integrated photodissociation cross-section in this interval contributes minimally to the total rate, except in the cases of extremely hot radiation sources. Near the photoionization limit, the photodissociation rate also decreases as it begins to compete with the photoionization process. Consequently, we supplement our results with the room-temperature Leiden cross-sections (J. B. Nee & L. C. Lee 1986) for the 116–135 nm spectral range, neglecting temperature effects in this specific region.

4.2 Photodissociation rates

The photodissociation rates [(photons) s^{-1} molecule $^{-1}$] are computed from our computed photodissociation cross-sections $\sigma(\lambda; T)$ and an incident radiation field $F(\lambda; T)$ as follows

$$k(T) = \int F(\lambda) \sigma(\lambda; T) d\lambda, \quad (11)$$

for various light sources and temperatures. This yields the rate at which the molecule photodissociates subject to the incident radiation flux $F(\lambda)$. In this study, we compute the temperature dependent photodissociation rates for incident radiation fluxes

described by blackbody radiation, defined as

$$B_{\lambda}^N = \frac{8\pi c}{10^{13} \cdot \lambda^4} \frac{1}{\exp[hc/(\lambda kT)] - 1}, \quad (12)$$

where all the input quantities are in SI, and the units of B_{λ} are photons $\text{s}^{-1} \text{cm}^{-2} \text{nm}^{-1}$. Following the Leiden convention (A. N. Heays et al. 2017; H. R. Hrodmarsson & E. F. Van Dishoeck 2023) the spectral energy density of the flux $F(\lambda)$ between 91.2 and 200 nm is normalized to that of the Draine field (B. T. Draine 1978; $2.5895 \times 10^{-6} \text{W m}^{-2}$).

Fig. 14 presents our computed photodissociation rates for the SO radical across a range of molecular temperatures and radiation environments. The left panel shows rates computed using integral-normalized radiation fields to facilitate comparison with the temperature-independent Leiden rates (horizontal dashed lines). We observe excellent agreement between the Leiden values and our low-temperature data. However, the SO photodissociation rates exhibit a moderate temperature dependence; for blackbody radiation sources at $T_{\text{rad}} = 3000, 4000, 5000, 7500$, and $10\,000$ K, the fractional increase between the $T = 1$ K rate and the rate at $T_{\text{gas}} = T_{\text{rad}}$ is 14.04, 6.81, 4.06, 1.66, and 1.04, respectively.

In exoplanetary atmospheres, certain regions (e.g. the upper atmosphere) can exist in extreme non-LTE conditions. The left panel of Fig. 14 tracks the temperature-dependent rate for a fixed radiation temperature over molecular temperatures up to $10\,000$ K. Under these conditions, we observe huge increase factors from the $T = 1$ K baseline of 1197.11, 53.91, 10.70, 1.84, and 1.04 for the $T_{\text{rad}} = 3000$ to $10\,000$ K sources, respectively.

While the Draine field integral normalization (A. N. Heays et al. 2017; H. R. Hrodmarsson & E. F. Van Dishoeck 2023) yields radiation fields better suited for applications to the ISM, it allows for a standardized comparison of radiation temperature dependence across sources by removing the dependence on photon

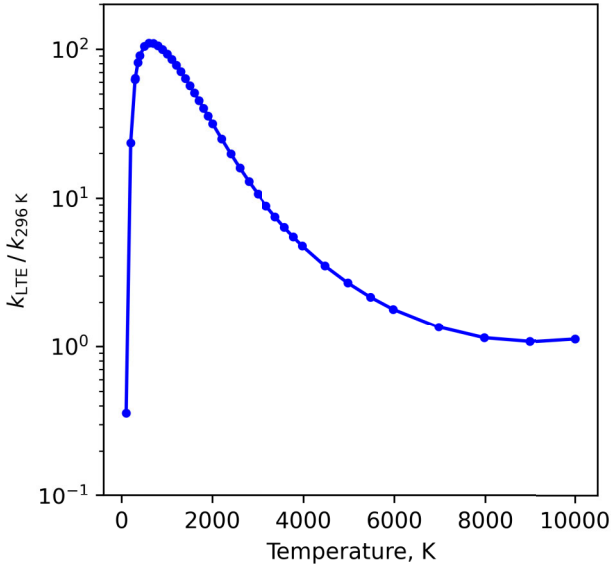


Figure 15. Ratio of our computed LTE rate (see text) to the rate computed with a gas temperature of 298 K for different radiation temperatures.

number. However, this does not reflect the physical reality of LTE environments like those found in deeper exoplanetary atmospheres. In LTE, the gas temperature equilibrates with the local radiation temperature ($T_{\text{gas}} = T_{\text{rad}}$). The right panel of Fig. 14 plots the LTE rate curve, revealing that while SO is stable on a cosmological time-scale below 1000 K, it exhibits extreme thermal sensitivity above the photodissociation onset at ~ 2000 K. We observe a four order of magnitude increase in the rate as the temperature reaches 4000 K, escalating to ten orders of magnitude at 10 000 K. This reveals the importance of treating temperature dependent photodissociation carefully in chemical models, especially in non-LTE cases where a cooler effective radiation field (< 3000 K) paired with a high molecular temperature can lead to even more drastic temperature effects. It is important to note that this specific analysis isolates the photodissociation rate and omits the competing effects of thermal dissociation. Under strict LTE conditions, SO may thermally dissociate at these extreme temperatures before a photon can be absorbed. However, the exact thermal dissociation rate depends heavily on the local gas density and composition, the modelling of which falls outside the scope of this work. A comprehensive investigation into the detailed balance and kinetic competition of SO would be highly relevant for understanding the proposed sulphur photochemistry in hot Jupiter atmospheres such as WASP-39b (Z. Rustamkulov et al. 2023; S.-M. Tsai et al. 2023b), and our temperature-dependent cross-sections provide the fundamental molecular data necessary for these future LTE (and non-LTE) studies.

Furthermore, we highlight the limitations of using low temperature cross-sections, such as the 296 K spectrum by L. F. Phillips (1981) adopted by Leiden, for diverse radiation environments. Fig. 15 illustrates the ratio between the true LTE rate in Fig. 14 and the rate obtained by integrating Leiden cross-sections with various radiation fields (with no field integral normalization). At lower radiation temperatures (100–1000 K), the Leiden-based rates are underestimated by a factor of 100, only approaching equivalence as T_{rad} nears 10 000 K.

Fig. 16 illustrates the comparison between the rates calculated using bound-bound (k_{b-b}) versus continuum photoabsorption (k_{b-u}) cross-sections. This comparison reveals that the long-wavelength photodissociation of SO is primarily driven by predissociation (bound-bound), rather than direct continuum photoabsorption as seen in other previously studied molecules. For a 3000 K blackbody flux, the contribution of predissociation ranges from 5 to 17 times that of continuum absorption across the molecular temperature range. This ratio decreases to approximately 2.5 for a 10 000 K radiation source. Out of all molecules in the ExoPhoto data base, SO is the second fastest dissociating molecule, surpassed only by CH. SO resembles CH in its lack of low energy repulsive electronic states within the FC region of the ground state and its abundance of quasi-bound states above the dissociation limit. Interestingly, Fig. 16 reveals k_{b-u} has a minimum at a molecular temperature of ≈ 100 K for all radiation temperatures, whereas k_{b-b} has a local maximum at this position for all integral normalized radiation fields. Their summation yields a total photodissociation rate which removes most of the temperature dependence in the rates up to $T \sim 100$ –298 K, where predissociation dominates the rate and drives the temperature dependence.

As suggested by A. Sokolov et al. (2025), the topology and positioning of electronic curves are the likely drivers of both the magnitude and temperature dependence of photodissociation rates. Our studies indicate that while bound-continuum cross-sections generally produce the strongest temperature dependence, the absolute level of photodissociation is determined by the extent of predissociation. This, in turn, depends on the number of coupled electronic states in the FC region. This is a feature shared by SO and CH, but less so in other molecules studied to date. SO is unique, however, in that both the magnitude and temperature dependence of its photodissociation rate appear to originate mostly from predissociation cross-sections. This is likely due to the distinct electronic character of the $B^3\Sigma^-$ discussed in Section 4. Another reason may be due to the lack of electronic curves above ~ 50000 cm^{-1} (as discussed in Section 2.6), which reduces the cross-section in the FUV spectrum. A. Sokolov et al. (2025) discuss, however, that the radiation flux is mostly flat in this region, except for hot radiation sources (e.g. $T_{\text{rad}} = 10000$ K), and contributes negligibly to the photodissociation rate and its temperature dependence.

The strong temperature dependence of the SO photodissociation cross-section has profound implications for the modelling of exoplanetary photochemistry, particularly for hot Jupiters such as WASP-39b (S.-M. Tsai et al. 2023a; D. Powell et al. 2024) ($T_{\text{eq}} \approx 1100$ K). At elevated molecular temperatures, the population of excited rovibrational states shifts the photodissociation threshold significantly towards longer wavelengths (e.g. initiating near 21016.25 cm^{-1} , or 475.82 nm, at 1100 K). Because the stellar flux of a G-type star like WASP-39 ($T_* \approx 5485$ K) is large at these optical wavelengths, the high temperature cross-section allows a substantially larger fraction of the incident photons to photodissociate the molecule. To quantify this effect, we computed the photodissociation rate assuming a blackbody stellar spectrum for WASP-39 and we find that utilizing our 1100 K cross-sections yields a 15 per cent increase in the SO photodissociation rate compared to using the room-temperature (296 K) cross-sections (Leiden assumption). Furthermore, this effect becomes drastically more pronounced for planets orbiting cool host stars, where the stellar emission peaks at longer wavelengths. For a simulated 3000 K host star, using our 1100 K cross-sections results

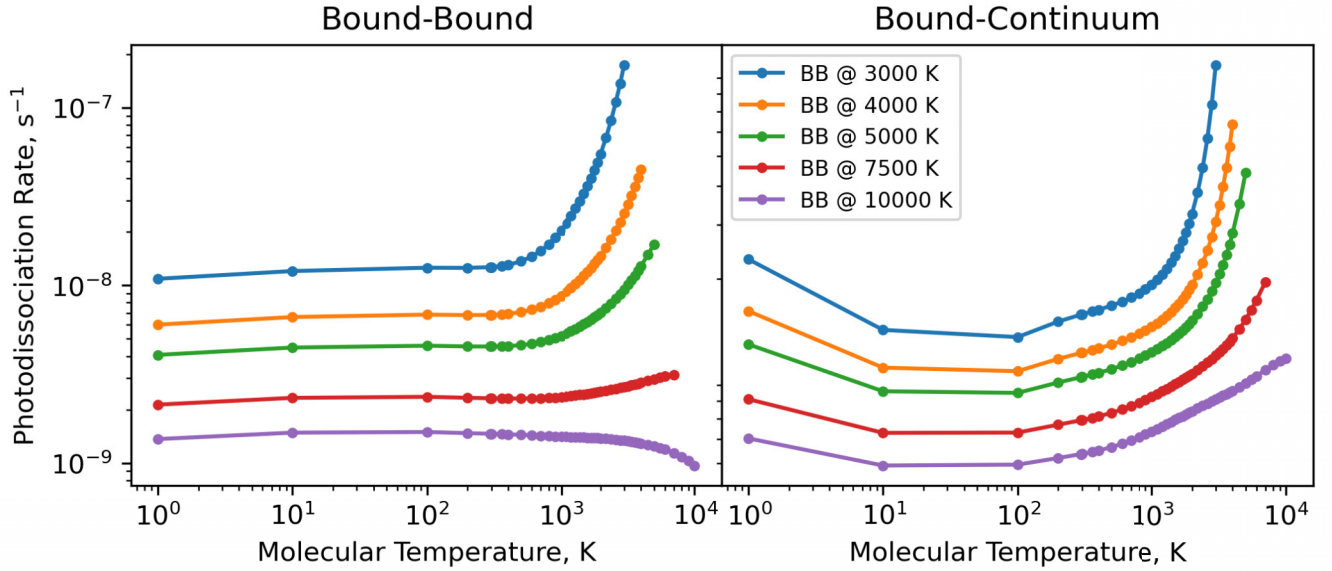


Figure 16. Contribution to the photodissociation rate by our calculated predissociated bound–bound cross-sections (left) and the direct continuum photoabsorption (right).

in a 72 per cent increase in the photodissociation rate compared to the 296 K baseline. Given that SO is a critical intermediate in the photochemical production of SO₂, such highly elevated photodissociation rate around cool stars could act as a significant bottleneck for SO₂ formation. These results highlight the absolute necessity of utilizing temperature-dependent cross-sections to accurately model photochemical networks and interpret atmospheric spectra, particularly for exoplanets orbiting M-dwarf stars.

5 CONCLUSIONS

We present calculated photodissociation cross-sections and an update to the SOLIS line list (<120 nm) of the SO radical called SOLUVIS. We compute a hybrid line list up to $J = 200$ from our previous high resolution line list, SOLIS, covering the $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, and $A^3\Pi$ (IR/Vis), a refined reduced model for the $B^3\Sigma^-$ and $C^3\Pi$ (UV), and an extended model covering also the $e^1\Pi$ and $C^3\Pi$ (FUV). We consider both type I predissociation of the $B^3\Sigma^-$ and $C^3\Pi$ states and direct continuum photoabsorption to the $C^3\Pi$.

The accuracy of our line list is validated by the excellent agreement found with experimental and semi-empirical spectra, as well as radiative and predissociative lifetimes from the literature. Furthermore, analysis of the PF demonstrates that for temperatures below 1000 K, the line list converges within the range of MARVEL coverage, thereby achieving experimental accuracy for these temperatures.

Photodissociation rates are computed for SO, where our analysis demonstrates that SO is an efficient photodissociating species. Unlike the other diatomics in the ExoPhoto data base, its near-threshold dissociation is primarily governed by predissociation rather than continuum absorption, a result of the high density of coupled electronic states in the FC region and the distinct (adiabatic) electronic character of the $B^3\Sigma^-$.

We find that SO photodissociation rates exhibit a moderate temperature dependence in integral normalized blackbody radiation fields, but this sensitivity escalates to ten orders of magnitude under LTE conditions as temperatures approach 10 000 K and the radiation field is not integral normalized. Crucially, the use of room-temperature Leiden cross-sections for atmospheric modelling can underestimate rates by a factor of 100 at lower radiation temperatures. These results highlight the necessity of employing temperature-dependent, high-resolution line lists to ensure accurate chemical modelling in both LTE and non-LTE exoplanetary environments.

Computed SOLUVIS photodissociation data are accessible through the ExoPhoto data base (Q.-H. Ni et al. 2025) at <https://www.exomol.com/exophoto>. Although ExoPhoto provides temperature-dependent cross-sections assuming LTE, our calculations are state-resolved. These state-specific data, which allow for the modelling of non-LTE environments (G. B. Mitev et al. 2025), form a significantly larger data set which is available from the authors upon request.

ACKNOWLEDGEMENTS

This work was also supported by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme through Advance grant no. 883830 and STFC grants UKRI/ST/B001183 and ST/Y001508/1. The work used the DiRAC Data Intensive service DiAL2.5 at the University of Leicester, managed by the University of Leicester Research Computing Service on behalf of the STFC DiRAC HPC Facility (www.dirac.ac.uk). The DiRAC service at Leicester was funded by BEIS, UKRI, and STFC capital funding and STFC operations grants. DiRAC is part of the UKRI Digital Research Infrastructure.

We would like to thank Armando Perri and Oleksiy Smola for their numerous discussions on spectra modelling, non-LTE modelling, and the stabilization methodology.

CONFLICT OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

DATA AVAILABILITY

The SOLUVIS DUO input files for bound and unbound line lists are given in the supplementary material.

The LTE temperature-dependent cross-sections for 16 gas temperatures ($\text{cm}^2 \text{ molecule}^{-1}$ versus nm) are available via the ExoPhoto data base <https://www.exomol.com/ExoPhoto>. Non-LTE cross-sections can be made available on request.

Precomputed opacity tables are available via www.exomol.com.

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SUPPLEMENTARY MATERIAL

Supplementary data are available at *MNRAS* online.

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