AN EXOMOL LINE LIST FOR SO: ROVIBRONIC SPECTRUM OF SULFUR MONOXIDE

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The work we present here is a diatomic molecule line list study on the molecule sulfur monoxide (SO), suitable for characterising exoplanetary atmospheres up to temperatures of 4000 K. The motivation of this project is to provide comprehensive line list data applicable to modelling high temperature spectra in environments such as e.g. exoplanetary atmospheres, where current spectroscopic databases provide only limited coverage. The new SO line list will be included into the ExoMol database.[a] A production of such a line list first includes the creation of a MARVEL[b] set of rovibroic energies, calculation of high-level *ab initio* potential energy curves (PECs), spin-orbit curves (SOCs), electronic-angular momentum curves (EAMCs) and transition moment dipole curves (TDMCs) using MOLPRO at MRCI level of theory and a solution of coupled ro-vibronic Schrödinger equations using the variational code DUO[c]. The PECs, SOCs and EAMCs are represented by analytical parametrised functional forms and refined by fitting to the MARVEL energies. A rovibronic line list for SO consists of energies, frequencies, Einstein coefficients and a partition function covering all electronic states up to 50 000 cm^{-1}, including $X\ ^3\Sigma^-$, $A\ ^3\Pi$, $A'\ ^3\Delta$, $A''\ ^3\Sigma^+$, $B\ ^3\Sigma^-$, $C\ ^3\Pi$, $a\ ^1\Delta$, $b\ ^1\Sigma^+$ and $c\ ^1\Sigma^-$. IR/Vis/UV absorption and emission spectra of SO for a set of temperatures are generated using the program ExoCross.[d]

[a] J. Tennyson et al. *J. Quant. Spectrosc. Radiat. Transf.*, 2020, **255**, 107228; *www.exomol.com*.

[b] T. Furtenbacher, A. G. Császár, J. Tennyson, MARVEL: measured active rotational-vibrational energy levels, J. Mol. Spectrosc. 245 (2007) 115–125.

[c] S. N. Yurchenko, L. Lodi, J. Tennyson, A. V. Stolyarov, *Comput. Phys. Commun.*, 2016, **202**, 262 – 275; publicly available at *https://github.com/Trovemaster/Duo*.

[d] S. N. Yurchenko, A. F. Al-Refaie, J. Tennyson, *Astron. Astrophys;*, 2018, **614**, A131; publicly available at *https://github.com/Trovemaster/ExoCross*.