

AB INITIO LINE LIST FOR DISULFUR MONOXIDE UP TO 1800 CM⁻¹

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The line list for the main isotopologue of disulfur monoxide (³²S₂¹⁶O) was variationally computed using both accurate *ab initio* potential energy (PES) and dipole moment surfaces (DMS). The applied *ab initio* PES¹ allows to describe the experimental band origins of ³²S₂¹⁶⁽¹⁸⁾O within the error of 0.5 cm⁻¹. The *ab initio* DMS was constructed *via* the finite difference approximation using the CCSD(T)/aug-cc-pV5Z approach. The final line list covers the 0-1800 cm⁻¹ region and contains more than one million transitions with the intensity cutoff value of 10⁻²⁵ cm/molecule. The simulated absorbances agree well with the available measurements, particularly, in the regions of the ν_2 (380 cm⁻¹)² and ν_3 (679 cm⁻¹)³ fundamental bands. The integrated intensities of the strongest cold and hot bands located in the 0-1800 cm⁻¹ region are presented.

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