From the quantum number dependence to a complete listing of sulfur dioxide self broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations

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Sulfur dioxide is one of the molecules included in the majority of the spectroscopic databases, given its relevance either in the Earth's atmosphere and in the interstellar medium. Indeed, it plays a relevant role in the chemistry of the Earth's atmosphere, directly entering in the sulfur cycle. Natural SO_2 origins from biomass burning and volcanic eruptions, nevertheless the main sources of atmospheric SO_2 arise from anthropogenic activities: once in the atmosphere, sulfur dioxide is one of the main causes of acid rains. Furthermore, SO_2 is of astrophysical importance, as it has been identified in the interstellar medium and in the Venus atmosphere.

In this contribution a complete database of sulfur dioxide self-broadening coefficients, for ground state- and ν_1 band-transitions, is compiled by joining experimental measurements to theoretical calculations. The laboratory measurements are carried out for a number of ro-vibrational lines of the ν_1 band, lying in the 9 μm atmospheric window as well as for 12 pure rotational transitions of the vibrational ground state. The former experiments have been carried out by using the tunable diode laser spectrometer at the Laboratory of Molecular Spectroscopy of Venice, while measurements in the ground state have been performed at the Laboratory of Millimeter/Submillimeter-wave Spectroscopy of Bologna by means of a frequency modulated computer-controlled spectrometer working in the 65 GHz - 1.6 THz frequency range. Theoretical calculations of broadening coefficients are performed employing a semiclassical formalism based on the ATC (Anderson - Tsao - Curnutte) approximation. By using the set of experimental data so obtained, in conjunction with the theoretical collisional decay rates, the quantum number dependence of the broadening coefficients is investigated and a complete line list of self broadening coefficients is generated for 1635 transitions in the quantum number range $0 \leq K_a \leq 16$, $0 \leq J \leq 16$.