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Rotational excitation of CS and SiO molecules by collisions with Helium

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Observations of molecular emission at millimeter and infrared wavelengths, supplemented by careful and detailed modeling, are powerful tools to investigate the physical and chemical conditions of astrophysical objects. The modeling of the line intensities requires comparison with model excitation calculations using radiative as well as collisional rates. In the relatively cold environments, collisional excitation is dominated by collisions with the most abundant neutral species, He and H₂.

We present here new 2D potential energy surfaces for the SiO-He and CS-He systems, calculated at r-distance frozen at their experimental minimum energy distance. Both are obtained at the CCSD(T) level using aug-cc-VQZ basis sets for the three atoms and supplemented by bond functions. Close coupling calculations of the collisional excitation cross sections of the rotational levels of SiO and CS by He are calculated from kinetic energies ranging from 0.1 to 1500 cm⁻¹. The propensity rules between rotational levels are studied. For SiO, ΔJ even cross sections are much larger than ΔJ odd cross sections. At the opposite, for CS, ΔJ odd cross sections are much larger than ΔJ even cross sections. Excitation rates among the 31 first rotational levels of SiO and CS are calculated for temperatures ranging from 5-300K.