The $\nu_2$ and $\nu_5$ fundamental bands of thionyl chloride (SOCl$_2$) were measured in the 420 cm$^{-1}$ - 550 cm$^{-1}$ region using the FT-Far-IR spectrometer exploiting synchrotron radiation on the AILES beamline at SOLEIL. A straightforward line-by-line analysis is complicated by the high congestion of the spectrum due to both the high density of SOCl$_2$ rovibrational bands and the presence of the strong $\nu_2$ fundamental band of sulfur dioxide produced by hydrolysis of SOCl$_2$ with residual water. To overcome this difficulty, our assignment procedure for the two isotopologues $^{32}\text{S}^{16}\text{O}^{35}\text{Cl}_2$ and $^{32}\text{S}^{16}\text{O}^{35}\text{Cl}^{37}\text{Cl}$ alternates between a direct fit of the spectrum, via a global optimization technique, and a traditional line-by-line analysis. The global optimization, based on an evolutionary algorithm $^a$, produces rotational constants and band centers that serve as useful starting values for the subsequent spectroscopic analysis. This work also helped to identify the pure rotational submillimeter spectrum of $^{32}\text{S}^{16}\text{O}^{35}\text{Cl}_2$ in the $\nu_2 = 1$ and $\nu_5 = 1$ vibrational states. A global fit gathering all the data of SOCl$_2$ from the microwave, submillimeter, and far-infrared spectral regions $^b$ $^c$ has been performed $^d$, showing that no major perturbation of rovibrational energy levels occurs for the main isotopologue of the molecule.

$^c$M. A. Martin-Drumel et al., J. Chem. Phys., 144(8), (2016), 084305  