THE SPECTROSCOPY AND STRUCTURE OF THIOPHOSGENE (Cl_2CS) IN ITS SINGLET A_2 STATE: A HIGH RESOLUTION STUDY OF THE ROTATIONAL STRUCTURE OF THE n $\rightarrow \pi^*$ TRANSITION

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BG test - The results of our recent line-by-line rotational analysis of the ring dye laser LIF jet spectrum of the $^1A_2 \leftarrow ^1A_1$ (n $\rightarrow \pi^*$) rovibronic transition of thiophosgene (Cl_2CS) will be presented. A total of four bands have been analyzed. An interesting feature of the spectrum is the axis-switching that occurs in the excited state of the $^{35}Cl_2CS$ and $^{35}Cl^{37}ClCS$ isotopomers. The excited state geometry has been determined from a fit to the least-squares determined rotational constants. The molecule is approximately 24° out-of-plane which is lower than that determined from earlier Franck-Condon type analyses of the vibrational structure. We attribut the discrepancy to the one-dimensional nature of the model calculations used in these previous studies.