ANALYSIS OF HIGH-RESOLUTION SPECTRA OF SiF_4 COMBINATION BANDS

M. A. MERKULOVA, *National Research Tomsk Polytechnic University, 30, av. Lenina, 634050 Tomsk, Russia*; **V. BOUDON**, *ICB, 9, av. Alain Savary, B.P. 47870, F-21078 Dijon, France*; **L. MANCERON**, *Synchrotron SOLEIL, AILES Beamline, L'Orme des Merisiers, BP48, F-91192 St-Aubin Cedex, France*

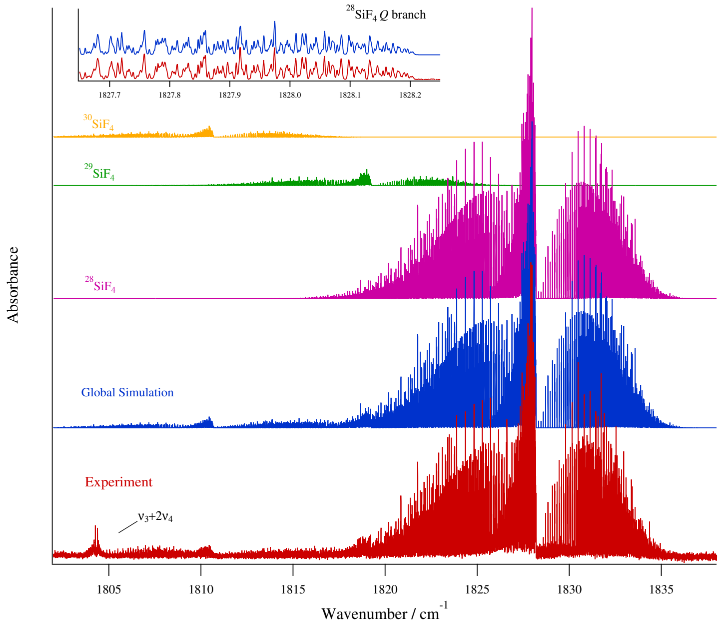
In this study, the spectrum of the silicon tetrafluoride molecule (SiF_4) was examined in five different combination band ranges. The energy structure of the vibrational states, specifically ($v_1 = v_3 = 1$), ($v_1 = v_4 = 1$), ($v_2 = v_3 = 1$), ($v_2 = v_4 = 1$), and very weak ($v_3 = v_4 = 1$), was determined. More than 8120 transitions were assigned with maximum rotational quantum number J_{max} values reaching up to 60 (up to 82 for ν_1+ν_3).

These results allowed for the precise determination of molecular parameters, with root mean square deviations for line positions as low as a few 10^{-4} cm^{-1}.

In the case of the ν_1+ν_3 band, the $^{29}SiF_4$ and $^{30}SiF_4$ isotopologues could also be assigned and fitted (figure below). These results will allow the calculation of hot bands like ν_3+ν_2-ν_2, $etc.$, in the regions of strong atmospheric absorption.

The obtained results hold significant value for their future application in the precise semi-empirical determination of the intramolecular potential function of tetrafluorosilane. Furthermore, they are of critical importance for the subsequent analysis of the line intensities associated with hot bands of this molecule. Part of this work was recently published[1].

[1]M. Merkulova, V. Boudon and L. Manceron, *J. Mol. Spectrosc.* **391**, 111738 (2023).



Overview of the ν_1+ν_3 spectrum, compared to the simulation for all isotopologues. The insert details a part of the Q branch region.