

DETAILED ANALYSIS OF THE INFRARED SPECTRUM OF SiF₄: AN UPDATE

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Silicon tetrafluoride (SiF₄) should be a normal trace component of volcanic gases. However, a better knowledge of spectroscopic parameters is needed for this molecule in order to derive accurate concentrations.

As explained last year, we undertook an extensive high-resolution study of its infrared absorption bands, for the three isotopologues in natural abundance: ²⁸SiF₄ (92.23 %), ²⁹SiF₄ (4.67 %) and ³⁰SiF₄ (3.10 %). We present here an update of this study. It includes a new global fit with consistent parameter sets for the ground and excited states (the Figure on the right presents the ν_4 bending fundamental region). In particular, all existing rotational line data have been included. The $2\nu_4$ band of ²⁸SiF₄ could also be analyzed in detail. A first rough estimates of the dipole moment derivative for the ν_3 band has been performed, leading to an integrated band intensity which is consistent with literature values, around 680 km/mol. The isotopic dependance of band centers and Coriolis parameters has been studied, thanks to the formula presented in talk P4363.

