SILYL FLUORIDE: LAMB-DIP SPECTRA AND EQUILIBRIUM STRUCTURE

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Different isotopic species of sylil fluoride, namely $^{28}SiH_3F$, $^{29}SiH_3F$, and $^{30}SiH_3F$, have been investigated by means of rotational spectroscopy. In particular, the Lamb-dip technique has been employed for resolving the hyperfine structure (hfs) of rotational lines, which is mostly due to the fluorine nucleus. The high resolution of such a technique allowed us to obtain the hyperfine parameters to a very good accuracy. The experimental determination has been strongly supported by highly accurate quantum-chemical calculations of the hyperfine parameters involved (spin-rotation constants as well as direct spin-spin interaction constants), providing reliable values for those parameters experimentally non-determinable.

Furthermore, the combination of experimental ground-state rotational constants for different isotopic species with the corresponding calculated vibrational corrections has been considered to determine the equilibrium structure. This evaluation has been supplemented by pure ab initio determinations. More precisely, taking the coupled-cluster singles and doubles (CCSD) level augmented by a perturbative treatment of triple excitations (CCSD(T)) as starting point, extrapolation techniques as well as the inclusion of minor contributions, such as core-correlation effects and higher-excitation, have been considered for obtaining highly accurate results.