TWO EQUIVALENT INTERNAL ROTATIONS OBSERVED IN THE MICROWAVE SPECTRUM OF 2,6-DIMETHYLFLUOROBENZENE

SAFA KHEMISSI, HA VINH LAM NGUYEN, *CNRS UMR 7583, Université Paris-Est Créteil, Université de Paris, Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), Créteil, France*.

The microwave spectrum of 2,6-dimethylfluorobenzene, one of the six isomers in the dimethylfluorobenzene family, was measured using a pulsed molecular jet Fourier transform microwave spectrometer in the frequency range from 2 to 40 GHz. Quantum chemical calculations were performed at the B3LYP/6-311++G(d,p) and MP2/6-31G(d,p) levels of theory to obtain optimized molecular geometries. The latter level yielded values of the rotational constants which were in almost exact agreement with the experimental values, and had eased tremendously the spectral assignment. Due to the internal rotation of the two equivalent methyl groups, all rotational transitions split into quartets with separations of up to several hundreds of MHz. The splittings were analyzed and modeled using the *XIAM*[a] and the *ntop* code[b] to measurement accuracy. The deduced V_3 potential value of 206.4 cm^{-1} is in reasonable agreement with the values predicted by quantum chemistry.

---

[a]H. Hartwig, H. Dreizler, *Z. Naturforsch.* **51a**, 923, (1996).

[b]L. Ferres, W. Stahl, H.V.L. Nguyen, *J. Chem. Phys.* **151**, 104310, (2019).