The IR spectrum of DCCF in the 320 – 850 cm^{-1} region: bending states up to $v_4 + v_5 = 3$

M. Villa [a], E. Canè [a], L. Fusina [a], H. Bürger [b], and M. Litz [b]

[a] Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, viale del Risorgimento 4, 40136 Bologna (Italy), Tel.: +39-051-2093707, Fax: +39-051-2093690 , E-mail: mattia.villa3@unibo.it, elisabetta.cane@unibo.it, luciano.fusina@unibo.it

[b] Anorganische Chemie, FB C, Bergische Universität, D-42097 Wuppertal, Tel.: , Fax: , E-mail:

Infrared spectra of deuterated monofluoroacetylene, DCCF, have been recorded in the region between 320 and 850 cm^{-1} at an effective resolution ranging from 0.0024 to 0.0031 cm^{-1}. In total, 6650 rotation vibration transitions were assigned to 37 bands involving the bending states with $v_4 + v_5$ and $|l_4 + l_5|$, respectively, up to 3, allowing the characterization of the ground state and of 18 vibrationally excited states. The ν_5 bending fundamental has been studied for the first time. In addition, the difference band $\nu_3 \leftarrow \nu_4$ has been detected and analyzed. All the assigned transitions have been fitted simultaneously by adopting a model Hamiltonian which takes into account the vibration and rotation *l*–type resonances. Rotational transitions in the ground and in bending excited states reported in the literature have been included in the global analysis. The set of 57 derived spectroscopic parameters reproduces 6130 infrared and 90 microwave and millimetre–wave transitions satisfactorily with root mean square values of 5.3 $\times 10^{-4}$ cm^{-1}, and 77 kHz, respectively.