TORSIONAL SPLITTING IN THE ROTATIONAL SPECTRUM FROM 8 TO 650 GHz OF THE GROUND STATE OF 1,1-DIFLUOROACETONE

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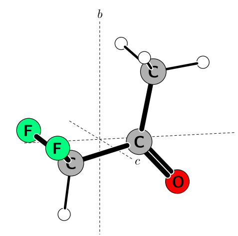
Measurements on the rotational spectrum of 1,1-difluoroacetone have been extended from the cm-wave region into the mm-wave region. Measurements between 150 GHz and 600 GHz were performed at Lille at room temperature. About 2000 transitions have been added to the known line listing for the ground state[a]. The range of J and K_{-1} values, for both the A and E torsional substates, now span 1 - 60 and 0 - 30, respectively. Analysis of the cm-wave spectrum was only possible using the Watson S-reduced Hamiltonian, with the A-reduction producing a poor spectral fit. For that analysis only quartic centrifugal distortion terms were required. With the newly recorded higher J and K_{-1} measurements it is necessary to expand the Hamiltonian to now include sextic and octic centrifugal distortion terms. This should allow us to extend the assignment to even higher J and K_{-1} and perhaps to shed more light into failure of the A-reduction Hamiltonian to achieve a satisfactory fit for the cm-wave transitions. The effective barrier to methyl group internal rotation has been determined more accurately.



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[a]G. S. Grubbs II, P. Groner, S. E. Novick and S. A. Cooke *J. Mol. Spectrosc.* **280** 21-26, 2012.