INTERNAL ROTATION ANALYSIS OF THE FTMW AND MILLIMETER WAVE SPECTRA OF FLUORAL (CF_3CHO)

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To protect atmosphere, hydrofluorocarbons (HFCs) are the current substituents of the dangerous CFCs and other ODS (ozone depleting substances).[b] Although HFCs are not ODS, they are potent greenhouse gases and, thus, they would be harmful to climate. Consequently, there is a keen interest on monitoring their reaction and the decomposition products in order to measure their effects. Fluoral (trifluoroacetaldehyde, CF_3CHO) is one of the stable decomposition products of several families of ODS substituents. Monitoring it in the atmosphere is hampered by the few spectroscopic data available in the literature. The rotational spectrum of fluoral from 8-40 GHz was measured previously,[c] however the performed analysis of the spectrum was rather limited due to difficulties in theoretical description. These difficulties reside mainly in the hindered internal rotation of the CF_3 group. Compared to acetaldehyde, in fluoral, the CF_3 group represents the major part of the molecular mass. Therefore, there is a strong coupling between the overall molecular rotation and the internal rotation of the top $\rho = 0.92$. As such, previously used principal axis method, where the axes remain unaffected by the large amplitude motion, is not fully suitable for the analysis. We present the analysis of new high resolution microwave and millimeter wave spectra of fluoral in the ranges 6-26 and 50-305 GHz, respectively, employing rho-axis method implemented in RAM36 program. The rotational distortional and internal rotational parameters that reproduce the spectral at experimental accuracy were determined for the ground state and several lowest excited torsional states.

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[b]Burkholder J.B. *et al.*, Chem.Rev., 2015, **115**, 3704

[c]Woods R.C., 1967, J. Chem. Phys., **46**, 4789