Trifluoroacetic Acid; r_0-Structure, Partial Substitution Structure and Deuterium Nuclear Quadrupole Coupling Studied by Molecular Beam Microwave Fourier Transform Spectroscopy and by *ab initio* Calculations

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We report the assignment and analysis of all stable monosubstituted isotopomers of trifluoroacetic acid. The ^{13}C and ^{18}O isotopomers were observed in natural abundance. The rotational constants and quartic centrifugal constants are presented. The rotational constants are used to derive a partial substitution structure and a complete r_0 structure for future comparison with the corresponding values in hydrogen bridged bimolecules containing trifluoroacetic acid as a subunit. The deuterium nuclear quadrupole coupling constants are derived from the hfs-splittings of low-J rotational transitions of the CF_3COOD isotopomer. The results of ab initio quantum chemical calculations are presented, which were carried out to assist in the assignment of the rotational spectra of the isotopomers and for comparison with the experimental molecular parameters.

Key words: Microwave Spectroscopy; Structure; D-hfs; Vibrational Averaging; *ab initio* Calculations.