^{2}H NUCLEAR QUADRUPOLE COUPLING OF ORGANIC ACIDS: A COMPARATIVE STUDY

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We present an investigation of the deuterium nuclear quadrupole coupling in a series of carbonic acids R-COOH: Among those, the acids with the groups R = CH_3 and R = CF_3 are two extreme cases for substituent effects on the charge distribution at the carboxyl group. The deuterium nuclear quadrupole coupling serves as a sensitive probe for the electric field gradient at the location of the acidic proton.
The rotational spectra and the quadrupole coupling hyperfine structures of several R-substituted carbonic acids R-COO^{2}H in the range of 6 to 26.5 GHz are reported.
Quantum chemical calculations were performed to determine the nuclear quadrupole coupling tensor of ^{2}H. The analysis of the nuclear quadrupole coupling in the rotational spectra provided experimental information on the tensors.