# $^2$H NUCLEAR QUADRUPOLE COUPLING OF ORGANIC ACIDS: A COMPARATIVE STUDY

JENS-UWE GRABOW, EIKE HENTROP, and DIETER H. SUTTER, *Chistian-Albrechts-Universiät, Institut für Physikalische Chemie, Abteilung Chemische Physik, Olshausenstrasse 40, D-24098 Kiel, Germany*.

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.