TWO DIMENSIONAL FOURIER TRANSFORM MICROWAVE SPECTROSCOPY: AUTO CORRELATION SPECTRUM OF 1-CHLORO-1-FLUORO ETHYLENE

CHANDANA KARUNATILAKA, KELLY M. HOTOPP, AMANDA J. SHIRAR, GIANA L. STORCK and BRIAN C. DIAN, *Department of Chemistry, Purdue University, West Lafayette, IN, 47907*.

Two dimensional (2D) microwave spectroscopy experiments were carried out to study the correlations between the rotational energy levels using a novel broadband chirped pulsed Fourier transform microwave spectrometer (CP-FTMW) system. The talk will mainly focus on two dimensional autocorrelation spectrum of 1-Chloro-1-Fluoro Ethylene (CFE). Connectivities and correlations between closely lying nuclear quadrupole hyperfine transitions (due to ^{35} Cl) were clearly observed in the spectra. Both diagonal and off-diagonal peaks were observed in the spectra, similar to COSY experiments in NMR [a]. Different pulse sequences were used to suppress the diagonal peaks. The large data set was worked up using a MathCAD program with a Kaiser Basel digital filter to obtain the frequency domain spectrum in both dimensions. 2D autocorrelation [b] and double quantum correlation experiments[c] were reported earlier on the CFE molecule with only 50 MHz bandwidth. In the present study, we extend this work to higher bandwidths (over 1 GHz) using CP-FTMW technique and monitored several rotational transitions at the same time.

[a] J. Jeener, Ampere International Summer School, Basko Polje, Yugoslavia, (1971)
[b] B. Vogelsanger, M. Andrist and A. Bauder, Chem. Phys. Lett., 144(2), (1988), 180-186
[c] B. Vogelsanger and A. Bauder, J. Chem. Phys. , 92(7), (1990), 4101-4114