THE THERMAL SELF-POLYMERIZATION OF METHYL METHACRYLATE — ROTATIONAL CHARACTERIZATION OF THE METHYL METHACRYLATE DIMER (IT'S NOT A COMPLEX!)

SVEN HERBERS, DANIEL A. OBENCHAIN, KEVIN G. LENGSFELD, HENNING KUPER, JENS-UWE GRABOW, JÖRG AUGUST BECKER, Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, Hannover, Germany.

Structural data from microwave spectra of monomers and oligomers of the methyl methacrylate system compared to theoretical predictions allows for accurate predictions of the structure and physical properties of higher oligomers or even polymers. The idea behind this project is to start with small building blocks and to successively increase the size of the oligomers in order to obtain more and more accurate predictions. Following the previous analysis of the monomer, this contribution focuses on the dimer of methyl methacrylate.

In the dimer phase of methyl methacrylate, which was subjected to a thermal self-polymerization process, the linear methyl methacrylate dimer was identified by means of rotational spectroscopy. The analysis was performed using the coaxially oriented beam-resonator arrangement Fourier-transform microwave (COBRA-FTMW) spectrometer. The dimer comprises three methyl rotors. Coupling of the methyl internal rotation to the overall rotation causes a complicated, challenging splitting of the rotational spectrum. The fact that only the two methoxymethyl groups contributed resolvable (>5kHz) splittings simplified the spectrum a little and a fit of molecular parameters to the experimental data was achieved with experimental accuracy utilizing the program XIAM.