ELECTRON-WITHDRAWING EFFECTS ON THE MOLECULAR STRUCTURE OF 2- AND 3-NITROBENZONITRILE REVEALED BY BROADBAND MICROWAVE SPECTROSCOPY

JACK B. GRANEEK, MELANIE SCHNELL, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*.

Nitrobenzonitrile consists of two electron-withdrawing groups, which have negative inductive and mesomeric effects on the phenyl ring resulting in interesting physical properties. The rotational spectra of 2- and 3-nitrobenzonitrile were recorded via chirped-pulse Fourier transform microwave spectroscopy in the frequency range of $2-8$ GHz. For both molecules, the main isotopologues and all isotopologues of the respective ^{13}C-, ^{15}N-, ^{18}O-monosubstituted species in their natural abundance were assigned. These assignments allowed for the structural determination of 2- and 3-nitrobenzonitrile via Kraitchman's equations as well as a mass-dependent least-squares fitting approach. Structural changes caused by steric interaction and competition for the electron density of the phenyl ring highlight how these strong electron-withdrawing substituents affect one another according to their respective positions on the phenyl ring.