HIGH RESOLUTION FIR–SPECTRUM OF OXETANE (TRIMETHYLENE OXIDE): ANALYSIS OF THE RING–PUCKERING FUNDAMENTAL NEAR 53 cm^{-1} AND OF SOME HOT BANDS

MANFRED WINNEWISSER, MARC KUNZMANN, and MICHAEL LOCK, *Physikalisch-Chemisches Institut, Justus-Liebig-Universität, D-35392 Gießen, Germany*.

Oxetane (C_3H_6O) is a four–membered ring molecule with a large–amplitude ring–puckering vibration, ν_{15}. The far infrared spectrum of this cyclic ether has been recorded between 50 and 160 cm^{-1} with a resolution of 0.00184 cm^{-1} (1/MOPD). Since room temperature spectra are not completely resolved, the sample was cooled to 200 K in order to obtain assignable rotation–puckering lines.

So far, the ${}^{Q}Q_{K_c}$ and ${}^{Q}R_{K_c}$ branches of the ring–puckering fundamental transition $v_{15} = 1 \leftarrow 0$ and of the hot band $v_{15} = 2 \leftarrow 1$ have been analyzed. From a least–squares fit using an *A*–reduced Watson Hamiltonian, the band origin of the fundamental transition is determined to be 52.920318(20) cm^{-1}. In addition precise rotational constants and centrifugal distortion parameters up to the sixth order for the ground and the first vibrational excited states are obtained. Preliminary results for some further hot bands will be discussed.