The Rotational Spectrum of (17O)Ketene

A. Guarnieri and A. Huckauf

Technische Fakultät der Christian-Albrechts-Universität zu Kiel,
Lehrstuhl für Hochfrequenztechnik, Kaiserstr. 2, D-24143 Kiel;
Institut für Physikalische Chemie der Christian-Albrechts-Universität zu Kiel,
Ludewig-Meyn-Str. 8, D-24098 Kiel, Germany

Reprint requests to Prof. A. G.; Fax: +49 431 880 6152; E-mail: ag@tf.uni-kiel.de

Z. Naturforsch. 56 a, 440–446 (2001); received April 9, 2001

The rotational spectrum of H2CC17O in the ground vibrational state has been investigated between 20 and 330 GHz. From 82 $R$-branch transitions a set of rotational constants and several centrifugal distortion constants could be derived, employing the Watson $S$-reduction formalism. The obtained rotational constants in MHz are: $A = 282071.6(223)$, $B = 10013.4764(28)$, $C = 9655.9118(24)$. The nuclear quadrupole coupling structure of the $J_{K_a K_c} = 1_{01} \leftrightarrow 0_{00}$ line has been recorded by means of molecular beam Fourier transform microwave spectroscopy allowing the determination of the nuclear quadrupole constant $\gamma_{aa} = -1.534(54)$ MHz (without considering the spin-rotation interaction). A recalculation of the $r_s$-structure has also been carried out, using the constants of the new isotopomer. The result agrees with the values reported by East et al. in 1995. This is, to our knowledge, the first reported investigation of the H2CC17O rotational spectrum.

Key words: Rotational Spectra; Structure; Ketene; Isotopomer.