THE COMPLETE MOLECULAR GEOMETRY OF SALICYL ALDEHYDE FROM ROTATIONAL SPECTROSCOPY

O. DOROSH, E. BIAŁKOWSKA-JAWORSKA, Z. KISIEL, L. PSZCZOLKOWSKI, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; M. KANSKA, T. M. KRYGOWSKI, Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland; H. MAEDER, Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Olshausenstrasse 40, D-24098 Kiel, Germany.

Salicyl aldehyde is a well known planar molecule containing an internal hydrogen bond. In preparing the publication of our previous report of the study of its rotational spectrum we have taken the opportunity to update the structure determination of this molecule to the complete \( r_{\text{SE}} \) geometry. The molecule contains 15 atoms and we have used supersonic expansion FTMW spectroscopy to obtain rotational constants for a total 26 different isotopic species, including all singly substituted species relative to the parent molecule. The \( ^{13}\text{C} \) and \( ^{18}\text{O} \) substitutions were measured in natural abundance, while deuterium substitutions were carried out synthetically. The \( r_{\text{SE}} \) determination requires the calculation of vibration-rotation changes in rotational constants from an \textit{ab initio} anharmonic force field, which necessitates some compromises in the level of calculation for a molecule of the size of salicyl aldehyde. For this reason we studied the five lowest vibrationally excited states, by using the combination of room-temperature mm-wave spectroscopy and waveguide Fourier transform cm-wave spectroscopy. The experimental excited state rotational constants were then used to calibrate the anharmonic force field calculation. The resulting \( r_{\text{SE}} \) geometry is compared with other types of geometry determination possible from this data, with emphasis on the effect of the near zero principal coordinate of the important \( \text{C}_2 \) atom.

\(^{a}\)Z.Kisiel et al., 61st OSU Symposium on Molecular Spectroscopy, The Ohio State University, Ohio 2006, RI-12.