

THE COMPLETE MOLECULAR GEOMETRY OF SALICYL ALDEHYDE FROM ROTATIONAL SPECTROSCOPY

O. DOROSH, E. BIALKOWSKA-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^a we have taken the opportunity to update the structure determination of this molecule to the complete r_e^{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 ¹³C and ¹⁸O substitutions were measured in natural abundance, while deuterium substitutions were carried out synthetically. The r_e^{SE} determination requires the calculation of vibration-rotation changes in rotational constants from an *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_e^{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 C₂ atom.

^aZ.Kisiel et al., 61st OSU Symposium on Molecular Spectroscopy, The Ohio State University, Ohio 2006, RI-12.