THE COMPLETE MOLECULAR GEOMETRY OF SALICYL ALDEHYDE FROM ROTATIONAL SPECTROSCOPY

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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 $r_e^{\mathrm{SE}}$ 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 substitued species relative to the parent molecule. The $^{13}$C and $^{18}$O substitutions were measured in natural abundance, while deuterium substitutions were carried out synthetically. The $r_e^{\mathrm{SE}}$ 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 $r_e^{\mathrm{SE}}$ 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 $C_2$ atom.

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