ROTATIONAL SPECTRUM, ELECTRIC DIPOLE MOMENT AND STRUCTURE OF SALICYL ALDEHYDE

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Salicyl aldehyde is a molecule with an intramolecular hydrogen bond that was first studied by rotational spectroscopy over 30 years ago.[a] We presently take advantage of the advances in this spectroscopic technique to considerably improve the knowledge of the molecular properties of salicyl aldehyde. The primary goal has been the determination of the complete molecular geometry of this molecule by rotational spectroscopy, with a minimum amount of synthetic isotopic substitution.

Broadband millimetre wave spectroscopy and $ab\ initio$ calculations were first used to establish accurate values of centrifugal distortion constants for fitting isotopic measurements. The use of the He/Ar carrier gas mixture, that has recently been found to be a useful tool for increasing the intensity of supersonic expansion FTMW spectra,[b] then allowed observation of singly substituted ^{13}C and ^{18}O isotopomers in natural abundance. Deuteration was performed in a way that allowed a mixture of isotopomers to be observed, and the results were fitted using the general structure fitting program STRFIT.[c] Deuterium nuclear quadrupole structure for the OD isotopomer was also analysed, and a precise determination of the electric dipole moment of salicyl aldehyde was made with the unique uniform-field Stark electrode arrangement developed in this laboratory.[d]

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[a] H.Jones, R.F.Curl, *J. Mol. Spectrosc.* **42**, 65 (1972)

[b] O.Desyatnyk, L.Pszczółkowski, S.Thorwirth, T.M.Krygowski, Z.Kisiel, $Phys.Chem.Chem.Phys.$ **7**, 1708 (2005)

[c] Z.Kisiel, PROSPE – Programs for Rotational Spectroscopy, `http://www.ifpan.edu.pl/~kisiel/prospe.htm`

[d] Z.Kisiel, J.Kosarzewski, B.A.Pietrewicz, L.Pszczółkowski, $Chem.Phys.Lett.$ **325**, 523 (2000).