THE STRUCTURE OF 4-METHYLPHENOL AND ITS WATER CLUSTER REVEALED BY ROTATIONALLY RESOLVED UV-SPECTROSCOPY USING A GENETIC ALGORITHM APPROACH.

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The structure of 4-methylphenol (p-cresol) and its binary water cluster has been elucidated by rotationally resolved laser induced fluorescence spectroscopy. The electronic origins of the monomer and the cluster are split into four subbands by the internal rotation of the methyl group and of the hydroxy group in case of the monomer and the water moiety in case of the cluster. From the rotational constants of the monomer the structure in the S_1-state could be determined to be distorted quinoidally.
The structure of the p-cresol-water cluster is determined to be translinear, with a OO hydrogen bond length of 290 pm in the electronic ground state and of 285 pm in the electronically excited state similar to the hydrogen bonded phenol-water cluster.