THE ROVIBRONIC SPECTRUM OF P-CYANOPHENOL

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The rotationally resolved vibronic origin spectrum of p-Cyanophenol (1-Hydroxy-4-Cyano-benzene) at 35547.46 cm^{-1} has been examined. The spectrum could be fit using a semi-rigid rotor hamiltonian with pure *b*-type selection rules. The inertial defects indicate that the molecule is planar in both excamined electronic states. In the spectrum of the parent molecule phenol, the internal rotation of the OH-group causes a splitting of the rotational lines of 56 MHz.[b] No such splitting could be observed in the p-Cyanophenol spectrum, indicating that it must be smaller than 15 MHz to fall within the observed linewidth.
The results of *ab initio* geometry optimizations and the theoretically determined torsional barries are compared to the experimental data. The influence of the para-substituent onto the internal rotation potential of the phenolic OH-group is discussed.

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