STATE LABELING SPECTROSCOPY: A NEW INSIGHT INTO INTERMOLECULAR VIBRATIONS AND TORSION OF THE WATER MOIETY IN PHENOL$(H_2O)_1$

MICHAEL SCHMITT, CHRISTOPH JACOBY and KARL KLEINERMANNS , *Institut für Physikalische Chemie und Elektrochemie I, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany.*

Intermolecular vibrations and their tunneling (torsional) symmetries have been assigned in the electronically excited state S_1 of phenol$(H_2O)_1$ and its deuterated isotopomers by resonant two photon ionization with time of flight mass analysis and spectral hole burning for state labeling. The abundance of transitions in the low frequency region between the electronic origin of the cluster and the stretching vibration can be traced back to the existence of torsional states of different symmetry, which split all vibrational modes. Based on the results of the hole burning spectra all transitions in the region of the intermolecular vibrations could be attributed to one of the symmetry species in question for the isotopically substituted phenol$(H_2O)_1$-clusters. The torsional splitting of all electronic origins could be determined with an accuracy of 0.1 cm^{-1}. A barrier to the internal rotation of the water moiety in the cluster could be estimated to 145 cm^{-1} for the S_0 and 113 cm^{-1} for the S_1 state. In addition a reassignment of some of the intermolecular transitions could be given.