

INTERNAL DYNAMICS OF WATER ATTACHED TO A PHOTOACIDIC SUBSTRATE: HIGH RESOLUTION ELECTRONIC SPECTROSCOPY OF β -NAPHTHOL-WATER IN THE GAS PHASE.^a

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An understanding of the structure and internal dynamics of water attached to the photoacid β -naphthol is attainable through rotationally resolved electronic spectroscopy. Here, we present rotational constants for the 1:1 acid-base cluster in both S_0 and S_1 , which provide the location of water within the cluster, as well as the barrier height to internal rotation of water in each electronic state. The barrier height decreases slightly upon excitation, from 206 cm^{-1} in S_0 , to 182 cm^{-1} in S_1 . There is also little evidence of a large change in water location, orientation, or overall hydrogen bond length upon irradiation with UV light. Thus, a single water molecule has relatively little affect on the substrate photo-acidity measured in the liquid phase.

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