SPECTROSCOPY OF ATMOSPHERICALLY IMPORTANT RADICAL-WATER COMPLEXES

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We have calculated the absorption spectrum of some hydrogen bonded radical-water complexes in the atmospherically important near-infrared and visible region of the spectrum. We have tested our method for the water dimer and our calculated band positions and intensities agree well with recently recorded matrix isolation spectra. Results for the $H_2O{\cdot}HO$ and $H_2O{\cdot}HOO$ complexes are also presented. The spectral intensities were calculated using an anharmonic local mode model and ab initio calculated dipole moment functions. The absorption properties of the complex are quite different to those of the monomeric constituents. The hydrogen bonded OH-stretching transition undergoes a significant redshift. These redshifted transitions may be used for possible detection of these complexes in the atmosphere.