INFRARED SPECTRA OF WATER BENDING BANDS OF PROPYLENE OXIDE-WATER COMPLEXES: SEQUENTIAL SOLVATION OF A CHIRAL MOLECULE IN WATER

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Sequential solvation of propylene oxide (C_3H_6O), an prototypical chiral molecule, with water has been investigated using high resolution infrared spectroscopy and *ab initio* methods. In a number of low resolution studies,[a] the vibrational and vibrational circular dichroism spectral features at the water bending vibration region had been shown to be highly sensitive to the water solvation structures around propylene oxide in aqueous solution. The current study aims to provide quantitative information about solvation of a chiral molecule with water molecules at the molecular level and to provide the experimental benchmarks for calculations of vibrational frequencies in these larger molecular complexes. The high resolution infrared spectra of the propylene oxide-water complexes have been measured using a pulsed jet infrared spectrometer equipped with a room temperature external cavity quantum cascade laser and an astigmatic multi-pass cell. At least 6 bands have been observed from 1650 to 1680 cm^{-1}. Based on the previous microwave spectroscopic studies,[bc] these bands have been assigned to the blue-shifted water bending (ν_2) vibration modes associated with both the *syn*- and *anti*- conformers of the binary (C_3H_6O-H_2O) and ternary (C_3H_6O-$(H_2O)_2$) complexes. This report shows the power of high resolution infrared spectroscopy to study multi-conformers of relatively large organic molecule complexes produced in a jet expansion.

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[b] Z. Su, Q. Wen, and Y. Xu, J. Am. Chem. Soc., 128, 6755, (2006)
[c] Z. Su and Y. Xu, Angew. Chem. Int. Ed., 46, 6163, (2007)