VIBRATIONAL SPECTRA OF THE $H_5O_2^+$ COMPLEX FROM THEORETICAL CALCULATIONS

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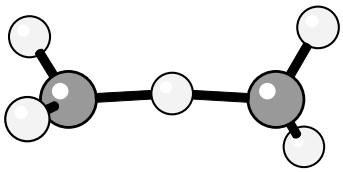

The $H_5O_2^+$ ion is abundant in the atmosphere, and in both the gaseous and condensed phases it plays an important role in proton-tranfer reactions. The very strong H-bond is believed to cause the large absorption observed in acid solutions.
In this talk we present theoretical investigations of the vibrational spectrum of this ion. We have calculated a potential surface for all of its 15 degrees of freedom by pointwise *ab initio* MP2 computations using a large basis set. Analytical expressions of various forms have been fitted to these points, and anharmonic vibrational frequencies have been calculated for parts of this surface using collocation methods. In particular, we suggest where the peak for the hydrogen-bonded OH stretching vibration can be found.

Time required: 15 min
Session in which paper is recomended for presentation: 8
Comment: *This abstract contains a graphic file, H5O2+.eps*