GEOMETRIES AND POTENTIAL ENERGY SURFACES OF THE HOO RADICAL IN RELATION WITH DOUBLE RENNER EFFECT: A THEORETICAL STUDY

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A preliminary account of the Double Renner effect in the HOO radical at high vibrational excitation was given at the 2003 Symposium.[a] In the $\hat{X}^2A$" and ^2A' electronic states of HOO, the proton orbits the OO moiety with two equivalent minima on each potential surface at bent geometries. At the two linear geometries HOO and OOH (which correspond to maxima on the potential energy surface) the two electronic states $\hat{X}^2A$" and ^2A' become degenerate as a Π state (TS1). The two equivalent minima on each surface of the $\hat{X}^2A$" and ^2A' states are separated by a maximum corresponding to a T-shaped geometry (TS2-^2A" and TS2-^2A').
To describe in more detail the effects of the tunneling between the two equivalent minima, we must extend the *ab initio* calculation of the potential-energy and dipole-moment surfaces. In particular, we need to improve the description of the potential energy and the dipole moment components for geometries near TS1 and TS2. Towards this end, we have been recalculating the geometries at the relevant stationary points and these surfaces at the level of core-valence MR-SDCI with aug-cc-pCVQZ (O) and cc-pVQZ (H) basis sets. We shall report the progress of this work at the meeting.

[a] *The 58th OSU International Symposium on High Resolution Molecular Spectroscopy*, 2003, Lecture WF12.