

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Water clusters  $(\text{H}_2\text{O})_n, n = 9-20$  in external electric fields: “Exotic” O-H stretches as precursors of breakdown**<sup>1</sup> RAJEEV PATHAK, Department of Physics, University of Pune, Pune, MH, India — Neutral, deformable clusters of water  $(\text{H}_2\text{O})_n [n = 9-20]$  subject to the highest tolerable “threshold” external electric fields on the verge of their breakdown exhibit some “exotic” O-H stretching modes in their infrared spectra. These normal vibrations, in which only *one or two* O-H stretchings contribute, emerge in the frequency range of 2327-2965  $\text{cm}^{-1}$ , markedly below the O-H stretching frequencies that commonly occur in the 3200-3600  $\text{cm}^{-1}$  region. These exotic modes essentially characterize the high degree of instability in these clusters immediately preceding their breakdown. On the other hand, a few clusters among those endowed with a  $C_n$  axis of symmetry remain “robust,” in that, they exhibit no major structural changes right up to their electric-field thresholds, wherein dominant stretches in the form of *collective* modes appear only beyond 3200  $\text{cm}^{-1}$ .

<sup>1</sup>Research Grant BCUD/RG, University of Pune is gratefully acknowledged.

Rajeev Pathak  
Department of Physics, University of Pune, Pune, MH, India

Date submitted: 05 Oct 2013

Electronic form version 1.4