Water clusters $(\text{H}_2\text{O})_n, n = 9-20$ in external electric fields: "Exotic" O-H stretches as precursors of breakdown

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 cm$^{-1}$, markedly below the O-H stretching frequencies that commonly occur in the 3200-3600 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 cm$^{-1}$.

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