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Edward M. Kosower

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Negative Infrared Bands – A New Phenomenon in the Vibrational Spectroscopy of Water Oligomers

By Edward M. Kosower*

School of Chemistry, Tel Aviv University, Tel Aviv 69978 Israel

*Inquiries may be addressed to kosower@post.tau.ac.il

Abstract

Infrared spectra of small amounts of water on the "hydrophobic" polymers, polyethylene(PE), polypropylene (PP) and polytetrafluoroethylene (PTFE), include many negative infrared bands that become positive with increasing temperature. The new species that the bands represent must arise through absorption of the incident radiation to form short-lived femtosecond states that disappear by (a) induced (Einstein) emission, thus leading to negative IR bands, or (b) fragmentation with loss of vibrational energy or (c) are replaced by an infrared excited state. In addition, we must note that polyethylene, polypropylene and polytetrafluoroethylene carry water! and many water oligomers (chair, boat, and prism hexamer) are easily observed.

Keywords

Negative IR absorption bands; Hydrophobic surfaces; Water; Thin films