

ANHARMONICITY OF NORMAL VIBRATIONS  
AND ITS INFLUENCE ON DEVIATIONS  
OF O—H BOND IN H<sub>2</sub>O MOLECULE

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S u m m a r y

The inverse problem of vibrational spectroscopy for an H<sub>2</sub>O molecule in the gaseous state and liquid water has been solved. The calculations for chemical bond deviations were carried out taking the anharmonicity of vibrations into account. The potential barrier height and the inversion frequency through the linear configuration of an H<sub>2</sub>O molecule have been evaluated for a number of vibrational states.