P5469: Large Amplitude Motions and π-Hydrogen Bonding in the Thiophene–Water Complex Characterized by Rotational Spectroscopy and Quantum Chemical Calculations

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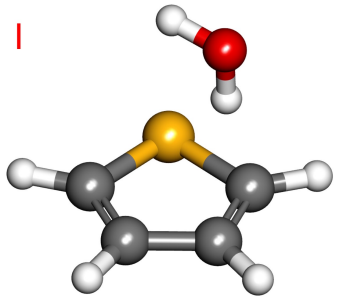
Motivation

Disagreement between experiment and theory

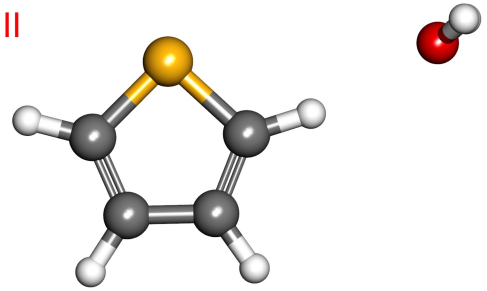
I



E (kJ mol^{-1}) = 0.0

Global minimum

II

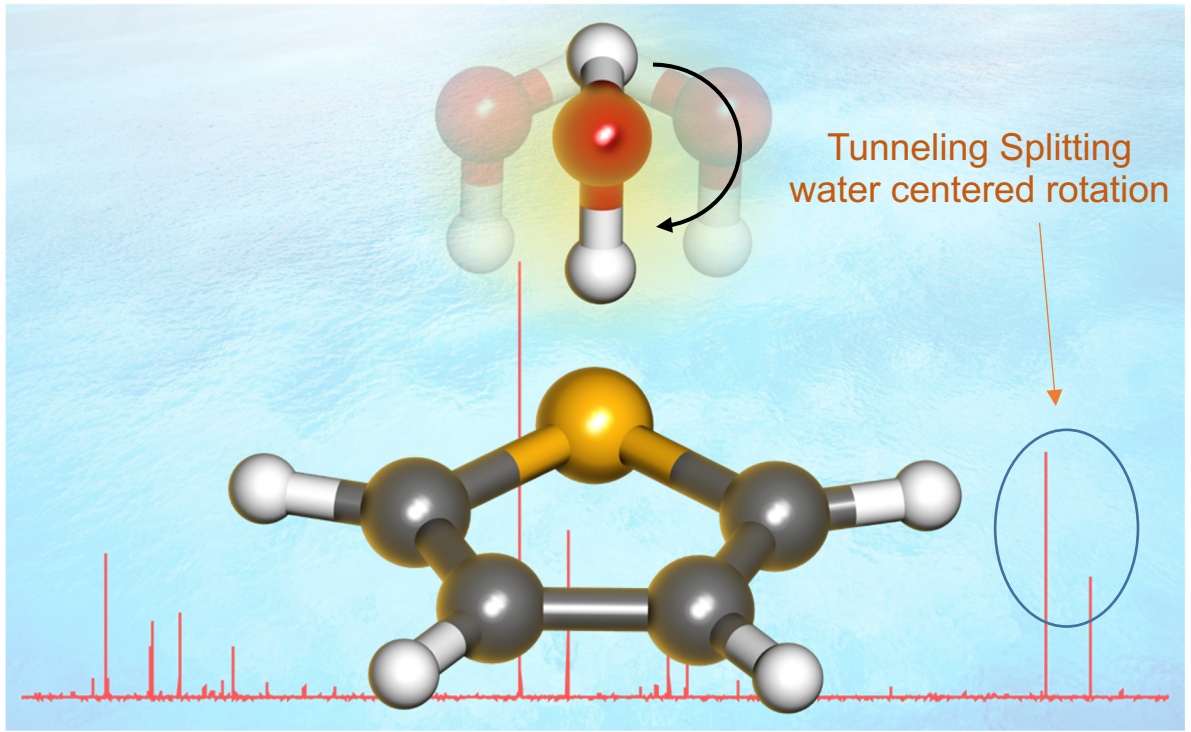


E (kJ mol^{-1}) = 2.4

Dominant features in Ar Matrix FTIR spectrum

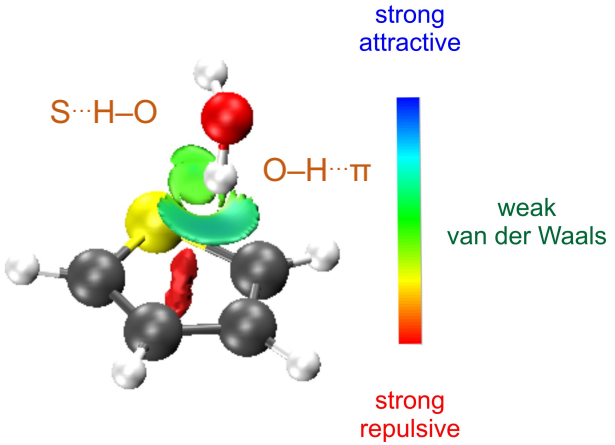
Our Findings

Highly averaged ground state structure



Supported by derived parameters, planar moments, selection rules and Kraitchman's analysis

Non-Covalent Interactions



Symmetry-Adapted Perturbation Theory

Electrostatic 48.6 %

Induction 14.6 %

Dispersion 36.8 %