

# H<sub>2</sub>O<sub>2</sub>-Ng Dynamics Predictions Using an Accurate Potential Energy Surface

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Based on *ab initio* calculations, our research group has built an analytical ground-state potential energy surface (PES) for hydrogen peroxide-noble gas (Ng) interactions, such as H<sub>2</sub>O<sub>2</sub>-He, H<sub>2</sub>O<sub>2</sub>-Ne, H<sub>2</sub>O<sub>2</sub>-Ar, H<sub>2</sub>O<sub>2</sub>-Kr, and H<sub>2</sub>O<sub>2</sub>-Xe complexes. It was verified in a previous study that the Ng presence does not affect the equilibrium values of the H<sub>2</sub>O<sub>2</sub> dihedral angles. This happens because the H<sub>2</sub>O<sub>2</sub> intramolecular barriers have much higher energies than the atom-bond interaction within these complexes. From this point of view, it is reasonable to consider the H<sub>2</sub>O<sub>2</sub> system as a rigid rotor, frozen at its equilibrium configuration. To complete this previous study, we present in this work the torsional motion for the H<sub>2</sub>O<sub>2</sub> isolated system, the vibration-rotation energy levels and spectroscopic constants for hydrogen peroxide-noble gas using the aforementioned PES. The predicted H<sub>2</sub>O<sub>2</sub> torsional motions are in a good agreement with both theoretical and experimental results available in the literature (Table I). Regarding H<sub>2</sub>O<sub>2</sub>-Ng ro-vibrational energies and spectroscopic constants, it is the first time that these calculations are presented in the literature. The current theoretical predictions are expected to be useful in the future experimental investigations.

TABLE I: Band frequencies (cm<sup>-1</sup>) for H<sub>2</sub>O<sub>2</sub> molecule. The differences among the experimental data (Exp1) and theoretical results are shown in parentheses.

Bands	Exp1.[1]	This work	Theor1.[2]	Theor2.[3]	Exp2.[4]
B1	11.43	11.52(0.09)	11.28(0.15)	11.03(0.40)	11.4372
B2	198.57	197.39(1.18)	199.13(0.56)	–	–
B3	370.70	372.31(1.61)	–	371.37(0.67)	370.8932
B4	557.84	558.18(0.34)	559.17(1.33)	–	–

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