PSEUDOROTATION IN TETRAHYDROFURAN: SPECTROSCOPIC AND MODEL POTENTIAL ANALYSIS

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The previously reported rotational structure of the $n = 0 \rightarrow n = 2$ pseudorotational band observed in the region of 182-335 GHz has been analyzed together with the data available from microwave measurements. A total of 280 transitions in the microwave and submillimeterwave region were globally fit to the Hamiltonian that we proposed earlier. The molecular parameters obtained from this fit are consistent with those recently reported from microwave measurements of the 6 lowest pseudorotational states. We have attempted to use the totality of the available experimental data to develop an empirical model of the potential surface along the pseudorotational path. \textit{Ab initio} calculations were also used to describe the potential surface along the pseudorotational path. The results of the modeling and comparisons between \textit{ab initio} and empirical surfaces will be discussed.

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