PSEUDOROTATION IN TETRAHYDROFURAN: SPECTROSCOPIC AND MODEL POTENTIAL ANALYSIS

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The previously reported[a] 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[b]. A total of 280 transitions in the microwave and submillimeterwave region were globally fit to the Hamiltonian that we proposed earlier.[a] The molecular parameters obtained from this fit are consistent with those recently reported from microwave measurements of the 6 lowest pseudorotational states.[c] 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. $Ab\ initio$ calculations were also used to describe the potential surface along the pseudorotational path. The results of the modeling and comparisons between $ab\ initio$ and empirical surfaces will be discussed.

[a] D.Melnik S.Gopalakrishnan, T.A.Miller, Rebecca A.H.Butler, and F.C.De Lucia, 55th International Symposium on Molecular Spectroscopy
[b] R. Meyer, J. C. Lopez, J. L. Alonso, S. Melandri, P. G. Favero, and W. Caminati J. Chem. Phys, 111, 7871 (1999)
[c] A.H.Mamleev, L.N.Gunderova, and R.V.Galeev, J.Struct.Chem, 42,365 (2001)