ROTATIONAL SPECTRUM OF NEOPENTYL ALCOHOL, $(CH_3)_3CCH_2OH$

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The rotational spectrum of neopentyl alcohol (2,2-dimethyl-1-propanol, $(CH_3)_3CCH_2OH$) has been investigated for the first time. This molecule differs from ethanol only in having the ^{t}Bu group instead of the methyl group, and is likewise anticipated to exhibit two spectroscopic species, with $trans$ and $gauche$ hydroxyl orientation. Quantum chemistry computations predict the $trans$ to be the more stable species. Rotational transitions of both species have now been assigned in supersonic expansion cm-wave FTMW experiment and in room temperature, mm-wave spectra up to 280 GHz. The supersonic expansion measurements with Ar carrier gas confirm that $trans$ is the global minimum species. The $trans$ spectrum is predominantly b-type, while the $gauche$ is predominantly a-type and the frequencies of rotational transitions in both species appear to be perturbed in different ways. The results from effective and from coupled Hamiltonian fits for neopentyl alcohol are presented, and are compared with predictions from $ab\ initio$ calculations.