COUPLED-STATE ANALYSIS OF ROTATIONAL TRANSITIONS OF THE GT, GG, and GG' CONFORMERS OF N-PROPANOL

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The rotational spectrum of the most stable Gt conformer of n-propanol has already been studied in some detail.[a] Rotational transitions in the Gg and Gg' conformers of n-propanol, which are related to Gt by rotation of the OH group, have also been assigned.[b]

Nevertheless, the single state analysis of the Gt conformer and the two-state analysis of the Gg-Gg' pair revealed various discrepancies, that suggested significant coupling between all three states. Attempts at a three-state Gt-Gg-Gg' fit were unsuccessful until a level crossing type perturbation between Gt and Gg energy levels was identified in the $FASST$ spectrum. This allowed a satisfactory three state solution to be located, and it became possible to account to within experimental accuracy for well over 6000 lines in the measured rotational spectrum. The resulting accurate relative energies of the pertinent conformers provide a benchmark for accurate $ab\ initio$ calculations, and are compared with results of a recent detailed computational study.[c]

[a] A.Maeda, et al. $Astrophys.\ J.\ Suppl.\ Series$ **162**, 428 (2006).
[b] Z.Kisiel, et al., RI14, 61st International Symposium on Molecular Spectroscopy (2006).
[c] K.Kahn and T.C.Bruice, $ChemPhysChem$ **6**, 487-495 (2005).