ASSIGNMENT OF GG, GG', TT and TG CONFORMERS IN THE $FASSST$ ROTATIONAL SPECTRUM OF N-PROPANOL

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Recent broadband measurements of the rotational spectrum of n-propanol up to 375 GHz resulted in determination of precise spectroscopic constants for the Gt conformer of this molecule.[a] This is most likely the most stable conformer, although four other conformers are predicted to be very similar in energy. Assignment of some of these in cm-wave rotational spectra has previously been reported, but it was not possible to extend that work directly to mm-wave spectra.

Application of graphical Loomis-Wood techniques built into AABS[b] and CAAARS[c] spectral analysis packages eventually allowed successful assignment of the remaining four conformers: Gg, Gg', Tt, and Tg n-propanol. It was realised that rotational energies in (Gg, Gg') and (Tt, Tg) pairs of conformers are highly coupled, but also amenable to description in terms of the Coriolis interaction mechanism. This allowed very precise determination of some energy level differences, such as $\Delta E(Gg' - Gg) = 3.035046(7)$ cm^{-1}. The assignment was checked against $ab\ initio$ calculations, and is supported by new, precise determinations of dipole moments of some conformers, which were carried out using supersonic expansion cavity-FTMW spectroscopy.

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[b] Z.Kisiel, L.Pszczółkowski, I.R.Medvedev, M.Winnewisser, F.C.De Lucia, E.Herbst, $J.\ Mol.\ Spectrosc.$ **233**, 231 (2005)
[c] I.R.Medvedev, M.Winnewisser, B.P.Winewisser, F.C.De Lucia, E.Herbst, $J.\ Mol.\ Struct.$ **742**, 229 (2005)