

EFFECT OF INTRAMOLECULAR DISPERSION INTERACTIONS ON THE CONFORMATIONAL PREFERENCES OF MONOTERPENOIDS

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The rotational spectra of several monoterpenoids have been reinvestigated with a 2-8 GHz chirped pulse FTMW spectrometer. Axial conformers, in addition to previously reported equatorial conformers^{a,b}, have been detected for carvone, perillaldehyde, and limonene. Observation of the ¹³C isotopologues of these monoterpenoids in their natural abundances allowed the determination of r_s and r_0 structures. Axial conformers are stabilised by dispersion interactions between the six-membered ring of the monoterpenoids and the isopropenyl group. Comparison of experimental data with ab initio and density functional calculations shows that an accurate description of dispersion interactions is still a challenge for theoretical methods.

^aJ. R. Avilés Moreno, F. Partal Ureña, J. J. López González and T. R. Huet, *Chem. Phys. Lett.*, 2009, 473, 17–20.

^bJ. R. Avilés Moreno, T. R. Huet and J. J. López González, *Struct. Chem.*, 2013, 24, 1163–1170.