

## CONFORMATIONAL ISOMERISM OF 1-IODOPENTANE

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The rotational spectrum of 1-iodopentane was measured over the 7-13 GHz frequency range with a chirped pulse Fourier transform microwave spectrometer revealing rotational transitions from a number of conformers.



This continues the group's work on how a large substituent, in this case an iodine atom, at the terminal position will affect the dihedral angles of the alkyl carbon backbone and what influence it will exert with continuing chain length. In keeping with last year's study of 1-iodobutane,<sup>a</sup> we find that the corresponding GAA conformer is the most abundant, and that while the nuclear quadrupole coupling tensor is poorly predicted by direct *ab initio* methods, scaling methods<sup>b</sup> allow very reasonable predictions to be obtained.

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<sup>a</sup>Arsenault E.A.; Obenchain, D.A.; Blake, T.A.; Cooke, S.A.; Novick, S.E; *J. Mol. Spectrosc.*, **2017** 335 17-22.

<sup>b</sup>Anticipated future communication with W. C. Bailey.