

1-IODOPENTANE, EXPERIMENTS AND CALCULATIONS

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The rotational spectra of two conformers, GAA and AAA, of 1-iodopentane have been recorded using both Fourier transform microwave cavity and chirp spectrometers. Iodine has a large nuclear electric quadrupole coupling tensor, χ , and is heavy enough to require a relativistic calculation for *ab initio* field gradient calculations. We will present a comparison of the experimental results, a calculation involving a clever scaling of the χ tensor,^a and a direct relativistic *ab initio* calculation.^b

^aW.C. Bailey and F.M. Gonzalez *J. Mol. Spectro.*, **651-653**, 689-695 (2003)

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