# IODINE: MANY ELECTRONS AND MUCH TO DISCUSS... THE NUCLEAR QUADRUPOLE COUPLING, NUCLEAR SPIN-ROTATION, CONFORMATIONAL ANALYSIS, AND STRUCTURAL DETERMINATION OF 2-IODOBUTANE

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The rotational spectrum of 2-iodobutane (sec-butyl-iodide) has been collected from 5.5-16.5 GHz using jet-pulsed Fourier transform microwave spectroscopy on both broadband[a] and Balle-Flygare cavity[b] instruments. Transitions belonging to three unique conformers were observed, namley the gauche-, anti-, and gauche′- species. All four $^{13}$C isotopologues of the gauche-2-iodobutane were observed. The complete nuclear quadrupole coupling tensor of iodine has been determined for all conformers and $^{13}$C isotopologues. A comparison between these nuclear quadrupole coupling tensors and those of similar iodine-containing molecules will be presented. Changes in the quadrupole coupling of iodine upon isotopic substitution will also be discussed. Additionally, isotopic substitution in conjunction with *ab initio* calculations allowed for both an $r_s$ and $r_0$ structural analysis of gauche-2-iodobutane.

[a]Brown, G. G.; Dian, B. C.; Douglass, K. O.; Geyer, S. M.; Shipman, S. T.; Pate, B. H. *Review of Scientific Instruments* **2008**, *79*, 053103.
[b]Balle, T.; Flygare, W. *Review of Scientific Instruments* **1981**, *52*, 33-45.