A STUDY OF THE CONFORMATIONAL ISOMERISM OF 1-IODOBUTANE BY MICROWAVE SPECTROSCOPY

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The rotational spectrum of 1-iodobutane was measured in a frequency range of 7-13 GHz, revealing a dense set of rotational transitions. Over 400 of the observed transitions were assigned to three different low energy conformational isomers. A previous low resolution microwave study[a] of 1-haloalkanes, including 1-iodobutane, confirmed that the three conformers present are the anti-anti, gauche-anti, and gauche-gauche species. From this high resolution study, the complete nuclear quadrupole coupling tensor of iodine was determined for each conformer. Rotational, centrifugal distortion, nuclear spin-rotation coupling constants will be discussed. Nuclear quadrupole coupling constants will also be presented and compared to other iodoalkane species.

[a]Steinmetz, W. E.; Hickernell, F.; Mun, I. K.; Scharpen, L. H. *J. Mol. Spectrosc.* **1977**, *68*, 173-182.