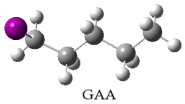
CONFORMATIONAL ISOMERISM OF 1-IODOPENTANE

SUSANNA L. STEPHENS, *Department of Chemistry, Wesleyan University, Middletown, CT, USA*; JOSHUA A. SIGNORE, *Chemistry , Wesleyan University , Middletown, USA*; DANIEL A. OBENCHAIN, *Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, Hannover, Germany*; ROBERT KARL BOHN, *Department of Chemistry, University of Connecticut, Storrs, CT, USA*; STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT, USA*; S. A. COOKE, *Natural and Social Science, Purchase College SUNY, Purchase, NY, USA*.

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,[a] 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[b] allow very reasonable predictions to be obtained.



GAA

[a] Arsenault E.A.; Obenchain, D.A.; Blake, T.A.; Cooke, S.A.; Novick, S.E; *J. Mol. Spectrosc.*, **2017** *335* 17-22.

[b] Anticipated future communication with W. C. Bailey.