BROADBAND CHIRPED-PULSE FOURIER-TRANSFORM MICROWAVE SPECTROSCOPIC INVESTIGATION OF THE STRUCTURES OF THREE DIETHYLSILANE CONFORMERS

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The rotational spectrum of diethylsilane has been assigned using broadband chirped-pulse Fourier-transform microwave (CP-FTMW) spectroscopy. Previously, Fourier-transform microwave rotational spectra were observed using a Balle-Flygare type instrument for the ^{28}Si isotopologues of the gauche-gauche, trans-gauche, and trans-trans conformers.[a] In the present study, a broadband microwave spectrum was obtained at the University of Virginia, taking advantage of the ability to perform deep signal averaging to increase the measurement sensitivity. To obtain a full structural determination of the conformers of this molecule, spectra for the ^{29}Si, ^{30}Si, and single ^{13}C substitutions for the gauche-gauche, the trans-gauche, and the trans-trans species were assigned. Substitution (r_s) structures and inertial fit (r_0) structures were determined and a comparison between the experimental and ab initio structures will be presented. For the ^{28}Si isotopologues, the percent differences between the experimental and ab initio rotational constants are less than 1.5% for the trans-trans and trans-gauche and are between 2.0 and 5.0% for the gauche-gauche conformer. The structural parameters will be compared between this molecule, diethylgermane and other silicon containing molecules and the relative abundances of the three conformers will be discussed.

[a] S.A. Peebles, M.M. Serafin, R.A. Peebles, G.A. Guirgis, and H.D. Stidham *J. Phys. Chem. A*, (2009), DOI: 10.1021/jp811049n.