

NUCLEAR QUADRUPOLE COUPLING IN SiH_2I_2 DUE TO THE PRESENCE OF TWO IODINE NUCLEI

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The rotational spectrum of diiodosilane was measured with a jet-pulsed, cavity Fourier transform microwave spectrometer over the frequency range 8.8 GHz to 15 GHz and assigned for the first time. The complete nuclear quadrupole coupling (NQC) tensors for both iodine nuclei were obtained for the ^{28}Si , ^{29}Si , and ^{30}Si isotopologues of diiodosilane. In addition to the nuclear quadrupole coupling constants (NQCCs), rotational constants, centrifugal distortion constants, and nuclear-spin rotation constants were determined for each silicon isotopologue. Subtle, yet unmistakable, changes in the NQCCs of iodine upon isotopic substitution will be examined. A r_0 structure of diiodosilane was also fit via isotopic substitution, leading to the determination of bond lengths and angles: $\text{Si}-\text{I} = 2.4236(19) \text{ \AA}$, $\text{Si}-\text{H} = 1.475(21) \text{ \AA}$, $\angle(\text{I}-\text{Si}-\text{I}) = 111.27(13)^\circ$, and $\angle(\text{I}-\text{Si}-\text{H}) = 105.9(19)^\circ$. These results will be compared to the results of a previous gas electron diffraction study.