

³³S NUCLEAR QUADRUPOLE COUPLING IN THIIRANE, METHYLTHIIRANE, 2,2-DIMETHYLTHIIRANE, AND ANTI-2,3-DIMETHYLTHIIRANE: HYPERFINE STRUCTURE IN THE ROTATIONAL SPECTRA AND AB-INITIO CALCULATIONS

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We present an investigation of the nuclear quadrupole coupling in a series of substituted thiiranes along with thiirane itself: The rotational spectra and the quadrupole coupling hyperfine structures of ³³S thiirane, ³³S methylthiirane, ³³S 2,2-dimethylthiirane, and ³³S anti-2,3-dimethylthiirane in the range of 7 to 22 GHz are reported.

Quantum chemical calculations on the MP4(QSD) level with basis sets of high local quality were performed to determine the nuclear quadrupole coupling tensor of ³³S. The analysis of the nuclear quadrupole coupling in the rotational spectra provided experimental information on the tensors.