

MICROWAVE SPECTRA OF THE TWO CONFORMERS OF PROPENE-3- d_1 AND A SEMIEXPERIMENTAL EQUILIBRIUM STRUCTURE OF PROPENE

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FT microwave spectra have been observed and analyzed for the S (in-plane) and A (out-of-plane) conformers of propene-3- d_1 in the 10-22 GHz region. Both conformers display splittings due to deuterium quadrupole coupling; for the latter one only, a 19 MHz splitting due to internal rotation of the partially deuterated methyl group has been observed. In addition to rotational constants, the analysis yielded quadrupole coupling constants and parameters describing the tunneling splitting and its rotational dependence. Improved rotational constants for parent propene and the three $^{13}\text{C}_1$ species are recently available.^a Use of vibration-rotation interaction constants computed at the MP2(FC)/cc-pVTZ level gave equilibrium rotational constants for these six species and for fourteen more deuterium isotopologues with diminished accuracy from early literature data. A semiexperimental equilibrium structure, r_e^{SE} , has been determined for propene by fitting fourteen structural parameters to the equilibrium rotational constants. The new r_e^{SE} structure compares well with an ab initio equilibrium structure computed with the all-electron CCSD(T)/cc-pV(Q,T)Z model and with a structure obtained using the mixed regression method with predicates and equilibrium rotational constants.

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