

THE ROTATIONAL SPECTRUM OF DEUTERATED ISOPROPANOL (CH₃)₂CHOD

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Isopropanol has already been investigated by microwave spectroscopy and has been confirmed to exist in both *trans* and *gauche*; the two equivalent *gauche* forms were found split by tunneling by 46 798.50 MHz.^a The observation was extended to the deuterated species that has a deuterium in the hydroxyl group, and the *trans* spectra were detected. However, the *gauche* spectra have eluded assignment, presumably because the tunneling splitting was comparable with the rotational energy, making the rotational spectrum complicated. In the present study we have employed a Fourier transform microwave spectrometer and have succeeded in unambiguously assign the *gauche* spectra, because the low temperature simplified the spectrum and because the deuterium nuclear quadrupole coupling effect resulted in hyperfine structure only for the spectra of the deuterated species. In an initial stage, we observed two lines for each of the four transitions: $1_{10} \leftarrow 0_{00}$, $1_{11} \leftarrow 0_{00}$, $2_{02} \leftarrow 1_{11}$, and $2_{12} \leftarrow 1_{01}$ with the splitting ranging from 8.5 MHz to 36.0 MHz. By carefully examining all the possible assignments of the two lines to the *symmetric* and *antisymmetric* states, we finally arrived at the tunneling splitting of about 4400 MHz, which was much larger than that previously estimated (about 2000 MHz). We then extended the assignment to other transitions of J up to 5, including some between the *symmetric* and *antisymmetric* rotational levels. As in the case of the parent species, these inter-state transitions were stronger than those within the *symmetric* or *antisymmetric* state. The main molecular parameters we obtained from the analysis are *symmetric* state: $A = 8198.9104$ (19), $B = 7998.3213$ (14), $C = 4611.6717$ (15), $\chi_{zz} = -0.1051$ (57), $\chi_{xx} - \chi_{yy} = -0.0437$ (27); *antisymmetric* state: $A = 8199.4366$ (17), $B = 7998.0368$ (20), $C = 4611.6876$ (20), $\chi_{zz} = -0.0987$ (54), $\chi_{xx} - \chi_{yy} = -0.0444$ (27); *symmetric/antisymmetric* cross terms: $R_{zx} = 180.330$ (13), $R_{xy} = 271.2791$ (60), $\chi_{zx} = -0.030$ (30), $\chi_{xy} = -0.143$ (39), $\Delta E = 4431.4581$ (27) in MHz with the standard deviations in parentheses.

^aE. Hirota, *J. Phys. Chem.* **83**, 1457 (1979)