

Microwave determination of the molecular structures and nuclear couplings of the methyl halides.

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Microwave Determination of the Molecular Structures and Nuclear Couplings of the Methyl Halides

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ABSTRACT

Accurate measurements on the pure rotation spectra of methyl chloride, bromide and iodide have been made with multiples of a 10 mc/sec. frequency monitored by station WWV. The measurements, with existing infra-red data, allow a complete determination of the structures of these molecules. The IB values in $\text{g/cm}^2 \times 10^{-40}$ are: 63.1138 for $\text{C}_{12}\text{H}_3\text{Cl}_{35}$, 64.1009 for $\text{C}_{12}\text{H}_3\text{Cl}_{37}$, 87.6835 for $\text{C}_{12}\text{H}_3\text{Br}_{79}$, 88.0180 for $\text{C}_{12}\text{H}_3\text{Br}_{81}$, 111.843 for $\text{C}_{12}\text{H}_3\text{I}_{127}$ and 117.848 for

$\text{C}_{13}\text{H}_3\text{I}_{127}$. The molecular dimensions obtained are: for methyl chloride,

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036, $\angle \text{HCH} = 110^\circ 15'$; for methyl iodide, $d_{\text{CH}}=1100$, $d_{\text{CI}}=2.139$, $\angle \text{HCH} = 110^\circ$

nuclear quadrupole couplings, $eQ(\frac{1}{2}V_{zz})$, are: for Cl_{35} , - 75.13 mc/sec.;

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for Cl37, - 59.03 mc/sec.; for Br79, 577.0 mc/sec.; for Br81, 482.0 mc/sec.; and for I127, - 1934 mc/sec. Second-order effects in the hyperfine structure were observed for methyl bromide and methyl iodide.

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Nuclear Data Sheets for A= 39, fractal leads to the actual pitch angle.

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