

The Nuclear Magnetic Resonance Spectrum and Conformation of Perfluorocyclo-octane

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THE use of high-resolution n.m.r. spectroscopy in the investigation of conformation and conformational inversion of cyclic molecules is well established and a summary of such studies has recently been published.¹ Some time ago² we examined the ¹⁹F spectrum of perfluorocyclo-octane in dilute solution in trichlorofluoromethane at 30.107 Mc./sec. At 33° c, the spectrum consists of a single sharp line 2.0 c./sec. wide at half-height.

Progressive lowering of sample temperature produces line-broadening followed by splitting into two signals of equal intensity separated by 25.5 c./sec., the low-field signal being broader. It was thought that the spectrum below T_c represented the separate signals from the "axially" and "equatorially" disposed nuclei of a regular crown conformation in which the differential broadening was attributed to dissimilar unresolved

