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## Spin-symmetry conversion in methyl rotors induced by tunnel resonance at low temperature

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### Abstract

Field-cycling NMR in the solid state at low temperature (4.2 K) has been employed to measure the tunneling spectra of methyl (CH<sub>3</sub>) rotors in phenylacetone and toluene. The phenomenon of tunnel resonance reveals anomalies in H-1 magnetization from which the following tunnel frequencies have been determined: phenylacetone,  $\nu(t) = 6.58 \pm 0.08$  MHz; toluene,  $\nu(t(1)) = 6.45 \pm 0.06$  GHz and  $\nu(t(2)) = 7.07 \pm 0.06$  GHz. The tunnel frequencies in the two samples differ by three orders of magnitude, meaning different experimental approaches are required. In phenylacetone the magnetization anomalies are observed when the tunnel frequency matches one or two times the H-1 Larmor frequency. In toluene, doping with free radicals enables magnetization anomalies to be observed when the tunnel frequency is equal to the electron spin Larmor frequency. Cross-polarization processes between the tunneling and Zeeman systems are proposed and form the basis of a thermodynamic model to simulate the tunnel resonance spectra. These invoke space-spin interactions to drive the changes in nuclear spin-symmetry. The tunnel resonance lineshapes are explained, showing good quantitative agreement between experiment and simulations. (C) 2014 AIP Publishing LLC.

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