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

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JOURNAL OF CHEMICAL PHYSICS
Volume: 140 **Issue:** 8
Article Number: 084302
DOI: 10.1063/1.4865835
Published: FEB 28 2014
View Journal Impact

Abstract

Field-cycling NMR in the solid state at low temperature (4.2 K) has been employed to measure the tunneling spectra of methyl (CH3) 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 +/- 0.08 MHz; toluene, nu(t(1)) = 6.45 +/- 0.06 GHz and nu(t(2)) = 7.07 +/- 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.

Keywords

KeyWords Plus: GROUP ROTATION; POLARIZATION; NMR; HYPERPOLARIZATION; SPECTROSCOPY; STATES

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Funding

Funding Agency	Grant Number
Royal Society	
Engineering and Physical Sciences Research Council	GR/R34189/01

View funding text

Publisher

AMER INST PHYSICS, CIRCULATION & FULFILLMENT DIV, 2 HUNTINGTON QUADRANGLE, STE 1 N O 1, MELVILLE, NY 11747-4501 USA

Categories / Classification

Research Areas: Chemistry; Physics

Web of Science Categories: Chemistry, Physical; Physics, Atomic, Molecular & Chemical

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000332485900025

PubMed ID: 24588164

ISSN: 0021-9606

eISSN: 1089-7690

Journal Information

Table of Contents: Current Contents Connect
Impact Factor: Journal Citation Reports

Other Information

IDS Number: AC4IZ

Cited References in Web of Science Core Collection: **25**

Times Cited in Web of Science Core Collection: **2**