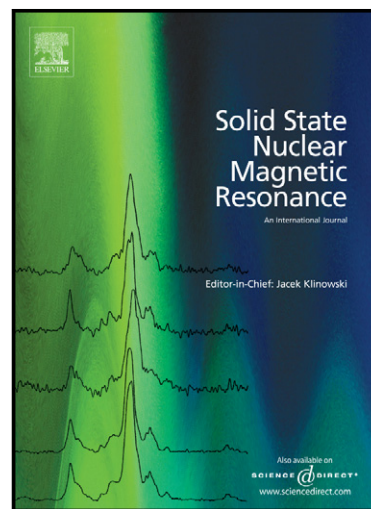


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Alexandra Faucher, Victor Terskikh, Roderick E. Wasylishen



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Feasibility of Arsenic and Antimony NMR Spectroscopy in Solids: An Investigation of Some Group 15 Compounds

Alexandra Faucher, Victor Terskikh^a and Roderick E. Wasylishen*

Department of Chemistry

Gunning-Lemieux Chemistry Centre

University of Alberta

Edmonton, AB

Canada T6G 2G2

^a Department of Chemistry, University of Ottawa, Ottawa, Ontario, K1N 6N5, Canada. E-mail: Victor.Terskikh@nrc-cnrc.gc.ca

* Author to whom correspondence may be addressed. Tel: 1-780-492-4336 E-mail: roderick.wasylishen@ualberta.ca

Abstract

The feasibility of obtaining ⁷⁵As and ^{121/123}Sb NMR spectra for solids at high and moderate magnetic field strengths is explored. Arsenic-75 nuclear quadrupolar coupling constants and chemical shifts have been measured for arsenobetaine bromide and tetraphenylarsonium bromide. Similarly, ^{121/123}Sb NMR parameters have been measured for tetraphenylstibonium bromide and potassium hexahydroxoantimonate. The predicted pseudo-tetrahedral symmetry at arsenic and the known trigonal bipyramidal symmetry at antimony in their respective tetraphenyl-bromide “salts” are reflected in the measured ⁷⁵As and ¹²¹Sb nuclear quadrupole coupling constants, $C_Q(^{75}\text{As}) = 7.8$ MHz and $C_Q(^{121}\text{Sb}) = 159$ MHz, respectively. Results of density functional theory quantum chemistry calculations for isolated molecules using ADF and first-principles calculations using CASTEP, a gauge-including projector augmented

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