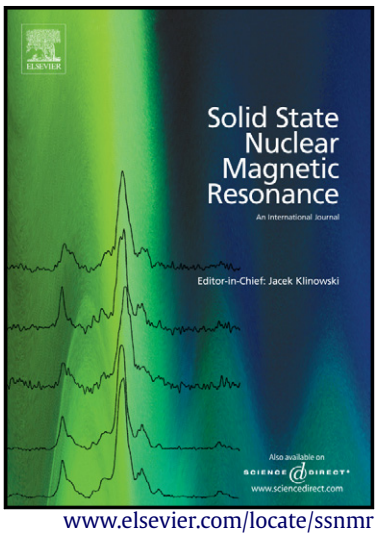

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Feasibility of Arsenic and Antimony NMR Spectroscopy in Solids: An Investigation of Some Group 15 Compounds

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Abstract

The feasibility of obtaining ^{75}As 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 ^{75}As and ^{121}Sb 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