

Theory of Nuclear Quadrupole Interactions of ^{14}N , ^{17}O , and ^{35}Cl Nuclei in *p*-Cl-Ph-CH-N=TEMPO

Junho Jeong^a, Tina M. Briere^b, N. Sahoo^{a,c}, T. P. Das^a, S. Ohira^e, K. Nishiyama^d, and K. Nagamine^{d,e}

^a Department of Physics, State University of New York at Albany, Albany, NY, 12222, USA

^b Institute of Materials Research, Tohoku University, Aoba-ku, Sendai, 984-8577, Japan

^c Department of Radiation Oncology, The Albany Medical College, Albany, NY 12208, USA

^d Meson Science Laboratory, Institute of Materials Structure Science, KEK, Tsukuba, Ibaraki, 305, Japan

^e Muon Science Laboratory, RIKEN, Wako, Saitama, 351-0198, Japan

Reprint requests to T. P. D.; Fax 1-(518)-442-5260

Z. Naturforsch. **57a**, 527–531 (2002); received May 17, 2002

Presented at the XVIth International Symposium on Nuclear Quadrupole Interactions, Hiroshima, Japan, September 9–14, 2001.

The nuclear quadrupole coupling constants and asymmetry parameters have been studied for the ^{35}Cl , ^{17}O , and ^{14}N nuclei in the molecular ferromagnet 4-(*p*-chlorobenzylideneamino)-TEMPO (2,2,6,6-tetramethyl-piperidin-1-yloxy) using electronic structures obtained by the Hartree-Fock procedure for the bare system and systems with trapped muon and muonium. Trends in the sizes of the coupling constants and asymmetry parameters for the various nuclei have been studied, and possible physical explanations have been proposed. For the systems with trapped muon or muonium, very substantial influences of the muon and muonium on the coupling constants and asymmetry parameters for the nuclei close to the trapping sites have been observed. The coupling constants and asymmetry parameters are found to be very different for the various nuclei, for the two cases where muon is trapped near chlorine and muonium near oxygen, indicating that, if experimental data were available to compare with theory, one could make conclusions about which of these two centers is responsible for the observed muon spin rotation frequency associated with the muon magnetic hyperfine interactions in these two trapped systems.

Key words: Chemical Ferromagnet; Nuclear Quadrupole Interactions; Hartree-Fock Theory.