Even-Odd Effect of ^{35}Cl Quadrupole Coupling Constants in Solid *n*-Alkylammonium Chlorides (C_5 - C_{10})

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^{35}Cl NMR spectra were measured using the highest-temperature solid phase of *n*-$C_xH_{(2x+1)}NH_3Cl$ and *n*-$C_xH_{(2x+1)}ND_3Cl$ ($x = 5-10$). The observed quadrupole coupling constants (e^2Qqh^{-1}) decreased upon heating in this phase, and significant frequency differences of *ca.* 20 – 30 kHz were detected between the -NH_3 and -ND_3 analogs. In the low-temperature range of this phase, the observed e^2Qqh^{-1} values for $x = 8, 10$ were larger than those for $x = 5, 7, 9$, which is attributable to the even-odd effect. Point-charge calculation was employed to explain this effect, in which the geometrical parameters and electric charge distributions of the cations were estimated using the B3LYP/6-31G* and B3LYP/6-31+G** method, respectively. The results show that the double-layer width between the Cl^- ions at the *2a* and *4f* sites strongly contributes to the e^2Qqh^{-1} value.

Key words: ^{35}Cl NMR Spectra; Theoretical Calculation of EFG; H-D Isotope Effect on Hydrogen Bonding; Even-Odd Effect.