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^{35}Cl NQR Spectra of 1,3-Dichloro-5,5-diphenylhydantoin and Related Compounds

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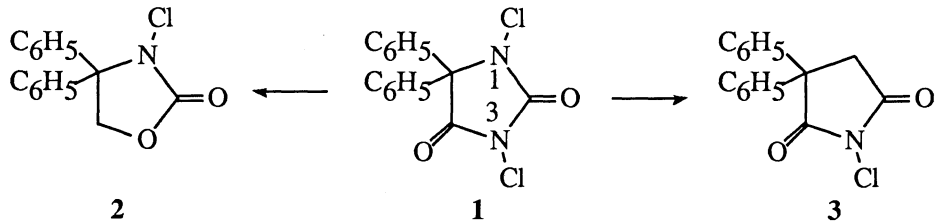
The ^{35}Cl NQR spectra were measured for 1,3-dichloro-5,5-diphenylhydantoin,**1**, *N*-chloro-4,4-diphenyl-2-oxazolidone,**2**, *N*-chloro-α,α-diphenylsuccinimide,**3**, and 1-chloro-5,5-diphenyl-3-methylhydantoin,**4**, at liquid nitrogen temperature. The resonance frequencies for these compounds were as follows: **1**, 55.019, 56.460 MHz; **2**, 52.914 MHz; **3**, 53.492, 53.717 MHz; **4**, 54.097 MHz.

It is an interesting attempt to measure ^{35}Cl NQR spectra of 1,3-dichlorohydantoin derivatives, because these compounds contain chemically nonequivalent two kinds of N-Cl bonds and give rise to two ^{35}Cl NQR signals. There have been only the reports of 1,3-dichloro-5,5-dimethylhydantoin in this group of compounds.[1,2] In the present study, ^{35}Cl NQR spectra of 1,3-dichloro-5,5-diphenylhydantoin and related compounds were measured and the assignment of two resonance signals of 1,3- dichloro-5,5-diphenylhydantoin was carried out by comparing the observed data.

It is thought that the natuer of the N-Cl bond adjacent to $(C_6H_5)_2$carbon in 1,3-dichloro-5,5-diphenylhydantoin, **1**, is close to that in a cyclic *N*-chloro amide derivative and the N-Cl bond between the carbonyl groups has a similar nature to that in a cyclic *N*-chloro imide derivative. The two kinds of N-Cl bonds in compound **1** are, namely, those at N(1) andN(3) are considered to correspond to those in *N*-chloro-4,4-diphenyl-2-oxazolidone, **2**, and *N*-chloro-α,α-diphenyl- succinimide, **3**, respectively.



2 **1** **3**

We used the Dean type self-quenched NQR spectrometer described previously.[3] 5,5-Diphenylsuccinimide were prepared according to literature.[4,5] The chlorination of these

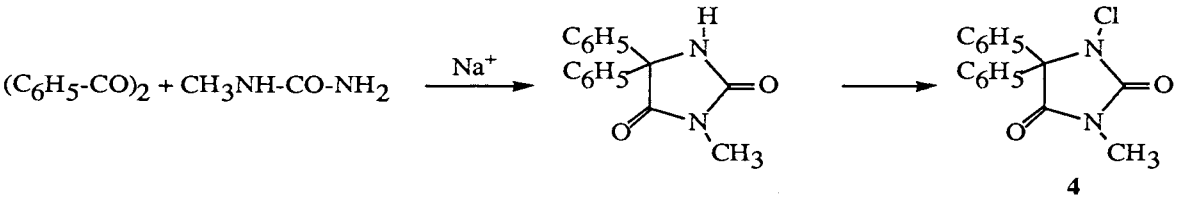
compounds was carried out by use of sodium hypochlorite solution.[6] All measurements were made at liquid nitrogen temperature.

The measured resonace frequencies are shown in Table 1. Compound **1** gave two signals at 55.019 and 56.460 MHz. These frequencies are higher than that of chlorine molecule. Compound **3**, although containing only one N-Cl bond, gave two resonance signals. The averaged frequency shown in parentheses in Table 1 is higher than 52.914 MHz observed in compound **2**. From this result, we can derive that the low frequency signal of compound **1** arises from the chlorine atom bonded to N(1) and that to N(3) gives rise to the high resonance frequency. These indicate that both the chlorine atoms on compound **1** are positively ionic and the inductive effect of two carbonyl groups in the vicinity of N(3) atom gives rise to an incerease in the resonance frequency due to N(3)-Cl bond compared with N(1)-Cl bond.

Table 1. ^{35}NQR Frequencies at Liquid Nitrogen Temperature

Entry	ν /MHz
1	55.019
	56.460
2	52.914
3	53.492
	53.717
	(53.604)
4	54.097

To make sure this assignment, 1-monochloro derivative of 5,5-diphenylhydantoin was prepared according to the reproted method of 1-chloro-5,5-dimethylhydantoin.[2] The product could unsuccessfully be obtained. Instead of this, 1-chloro-5,5-diphenyl-3-methylhydantoin, **4**, was prepared and its ^{35}Cl NQR signal was observed. The preparation is as follows ;



The ^{35}Cl NQR frequency of compound **4** was found at 54.091 MHz corresponding to the low frequency of comound **1**.

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