

$^{14}\text{N}$  NMR CHEMICAL SHIFT IMAGING

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The image of a phantom containing nitrogen compounds was obtained by  $^{14}\text{N}$  NMR method. The use of  $^{14}\text{N}$  chemical shift was successful in distinguishing the molecular species.

The NMR imaging technique using proton has been developed remarkably in the last decade and is already in the level of diagnostic use for the medical purposes. The difference in the  $^1\text{H}$  nuclear spin relaxation times is used to distinguish the tissues in vivo. Fundamental studies towards the NMR method combining tomography and spectroscopy have been reported using  $^1\text{H}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$  spectra of various simple compounds. The NMR imaging technique will become a useful tool for the in vivo study of distribution and dynamics including metabolism of drugs or simple compounds of physiological importance, and also in the field of material sciences. In this study, a method of  $^{14}\text{N}$  NMR was tested for the first time to construct the images of nitrogen compounds employing the information of chemical shift to distinguish these molecular species. The purpose of this report is to show the potential of the chemical shift method using the nuclei other than proton or nucleus of spin 1/2.

The  $^{14}\text{N}$  NMR spectra used for the image construction are shown in Fig. 1. Aqueous solution of ammonium chloride ( $\text{NH}_4\text{Cl}$ , saturated solution) and of acetylcholine bromide [ $(\text{CH}_3)_3\text{N}^+\text{CH}_2\text{CH}_2\text{OCOCH}_3 \cdot \text{Br}^-$ ,  $4 \text{ mol dm}^{-3}$ ] were used to constitute the phantom shown in Fig. 2 in a 10 mm NMR tube. The magnet of JEOL PS-100 NMR system and the home made pulse FT system<sup>4)</sup> operated at 7.2 MHz were used at ambient temperature (23 °C). The chemical shift difference of these two compounds was 168 Hz (23 ppm) with  $\text{NH}_4^+$  towards the upper field (Fig. 1a). The field gradient of  $4 \mu\text{T/mm}$  was applied from 4 directions to obtain the spatial information (Fig. 1b, c).

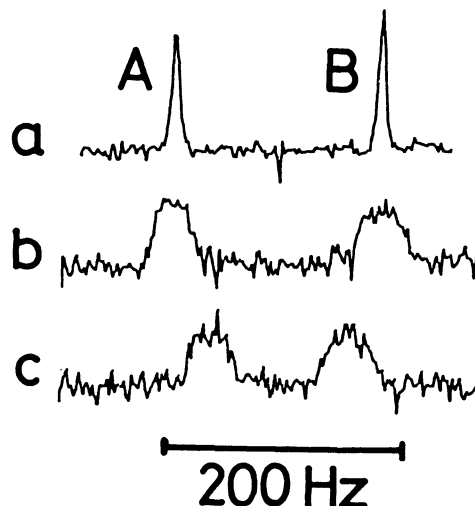


Fig. 1.  $^{14}\text{N}$  NMR spectra of A)  $\text{NH}_4\text{Cl}$  and B) acetylcholine bromide in the phantom. Pulse width  $43 \mu\text{s}$ , 512 scans.  
a) Without field gradient,  
b) field gradient applied to Y direction,  
c) field gradient applied to X direction.

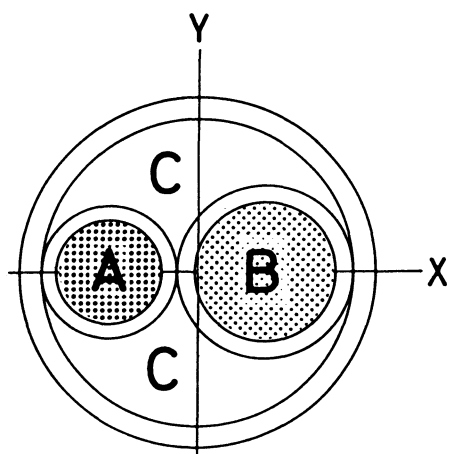
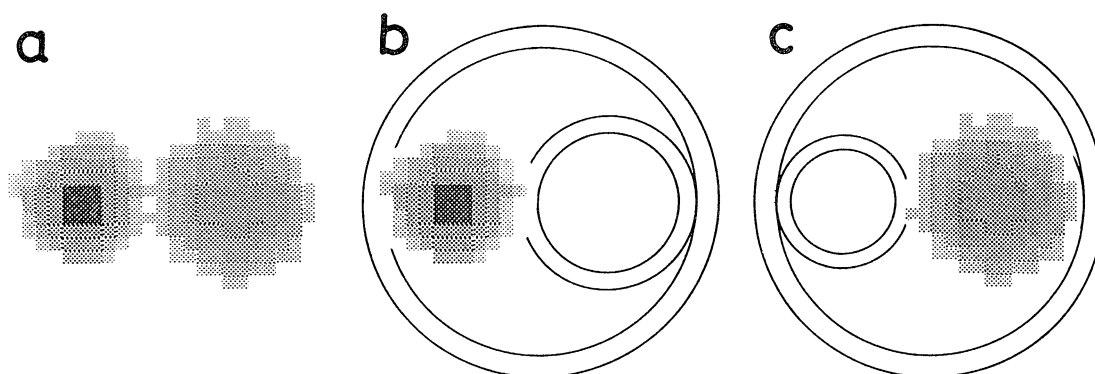


Fig. 2. The cross section of the phantom.  
A) NH<sub>4</sub>Cl, B) acetylcholine bromide, C) water.

Fig. 3. <sup>14</sup>N image of the phantom.  
a) Total <sup>14</sup>N density distribution,  
b) the image of NH<sub>4</sub><sup>+</sup>,  
c) the image of acetylcholine.



The image was obtained by projection-reconstruction method.<sup>5)</sup>

The results are shown in Fig. 3. The image has a sufficient resolution in spite of only 4 projections used for its reconstruction. This result provides a promising example of obtaining images of such compounds including the informations on molecular species.

The difficulties in <sup>14</sup>N NMR method lie in the low sensitivity due to the small magnetogyric ratio of the nucleus and the broadness of the signal due to nuclear quadrupole interactions. The present experiment is designed to show the possibility of application to such a nucleus. The wider chemical shift distributions of other nuclei compared to that of proton, e.g. 900 ppm from alkyl amine to nitroso compounds in the case of <sup>14</sup>N, will serve for easier distinction of molecular species and spatial resolution. It can be claimed here that this technique has a potential applicability in various field such as biochemistry, pharmaceutical and material sciences.

#### References

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