(Present Research at Toyota Riken)

Study on gas-phase NMR spectroscopy:

Preparation of cold ions in strong magnetic field and its application to gas-phase NMR spectroscopy

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Research background: Nuclear magnetic resonance (NMR) technique is widely used as a powerful tool to study the physical and chemical properties of materials. However, this technique is limited to the materials in condensed phases. To compensate these problems, recently, mass spectroscopy is extensively used in broad research fields including life and medical sciences. Since this method essentially only gives information on the mass number, and for further chemical information computer simulations are often required. Under these circumstances, a new extension of the NMR technique to the gas-phase molecular ions, which enable us to obtain rich information on the structure of the target ions with a mass-spectral sensitivity, becomes increasingly important for both fundamental and applied sciences

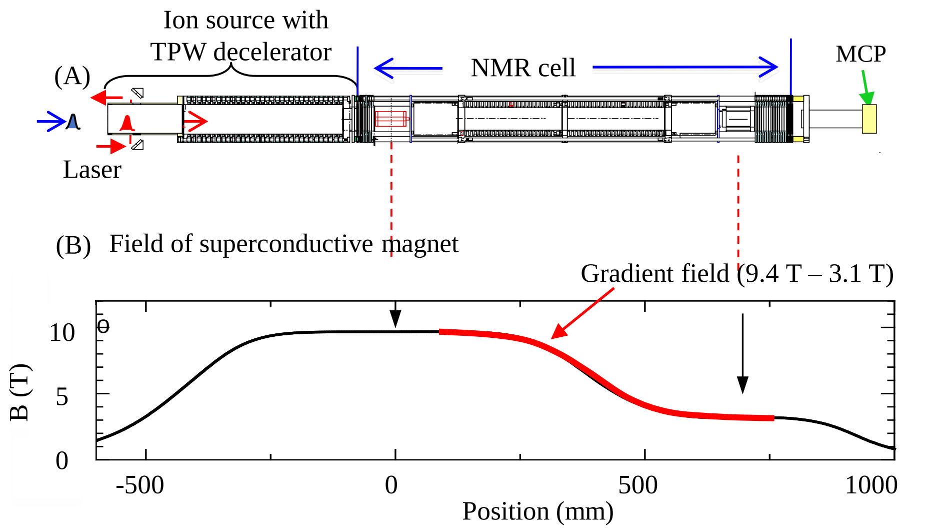
Principle of measurement, Progress report, and Future Plans: We proposed a new principle to detect NMR signals of gas-phase molecular ions based on a Stern-Gerlach type experiment in a Penning-trap type cell as shown in Fig. 1.[1,2] In this method, the cold molecular ions with a slow velocity and a very narrow velocity distribution width are introduced in the cell and their magnetic moments are probed by observing the modulation of their TOFs induced by flipping the nuclear spin with the coils placed at both ends of the cell. To realize the NMR detection, we constructed the gas-phase NMR apparatus for mass selected ions as shown in Fig. 2. We are developing the methods to prepare and manipulate cold molecular ions under the strong magnetic field. In the preliminary experiment, the ions are cooled by four steps. A supersonic molecular beam is used to precool the neutral molecules and photoionize it to form the cooled ion packet as cold as <2 K. Since the mean velocity of the ions is relatively high, the ions produced are cooled by the bunching and deceleration using a potential switch or a newly-developed traveling well potential (TPW) decelerator shown in Fig. 3. The ions decelerated are transferred to the NMR cell shown in Fig. 4 and cooled further by the velocity selection with mesh electrodes (ca. 30 mK) and finally with a velocity dispersion compensator (< 1 mK).[3] We also develop two sets of tuned circuits including coils as shown in Fig. 4, which can operate under an ultrahigh vacuum. The coils are placed at the higher (9.4 T) and the lower (3.1 T) homogeneous-field parts of the magnet as shown in Fig. 1 and generate two RF pulses at the Lamor frequency of the ^{1}H nuclei to rotate the magnetic moment by 180 degree. The two capacitors of each circuit can be adjusted from the outside of the vacuum chamber with rotational motion feedthroughs. These coils are calibrated by measuring the NMR signal of liquid water with a FT-NMR spectrometer.

At present, we are conducting the proof-in-principle experiment. The results on the basic performance of the present apparatus suggest that the first NMR signal for polyatomic ions will be detected in near future. We also plan to install an ion cyclotron resonance (ICR) cell at the upstream of the NMR cell in tandem to add a mass analysis function to this apparatus

Expected results, spread effects: From a viewpoint of basic science, the present apparatus allows us to extend the NMR measurement to the gas-phase molecular ions and to develop a new field of molecular science. By providing the mass analysis function, the apparatus can be utilized for chemical analysis in broad fields of sciences including life and medical sciences.

References: 1) K. Fuke, et al., Rev. Sci. Instrum. 83, 085106-1-8 (2012), 2) K. Kominato, K. Fuke, et al. IEEE Trans. Appl. Supercond.,20, 736 (2010). 3) K. Fuke, et al., Hyperfine Interactions, 236(1), 9-18.(2015).

Fig. 1 Schematic of gas-phase NMR apparatus



(NMR cell; details are in Fig. 4. TPW; traveling potential well)

Fig. 3 Ion source with multistage decelerator

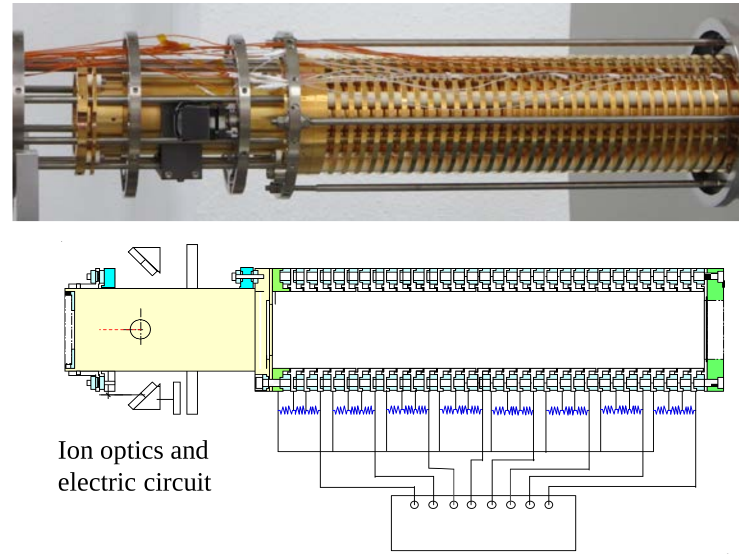
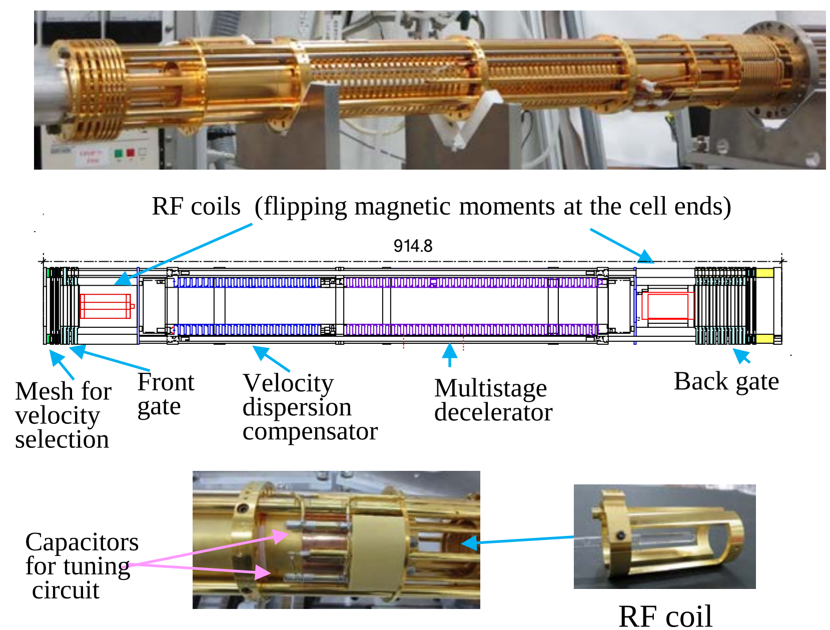


Fig.2 Photograph of gas-phase NMR apparatus

Magnet is 1.85 m in length and 2.2 m in height

Fig. 4 NMR cell (cooling and magnetic resonance)



Tuned circuit including RF coil