

Current Status of Microwave and Submillimeter-wave Spectroscopy in Japan

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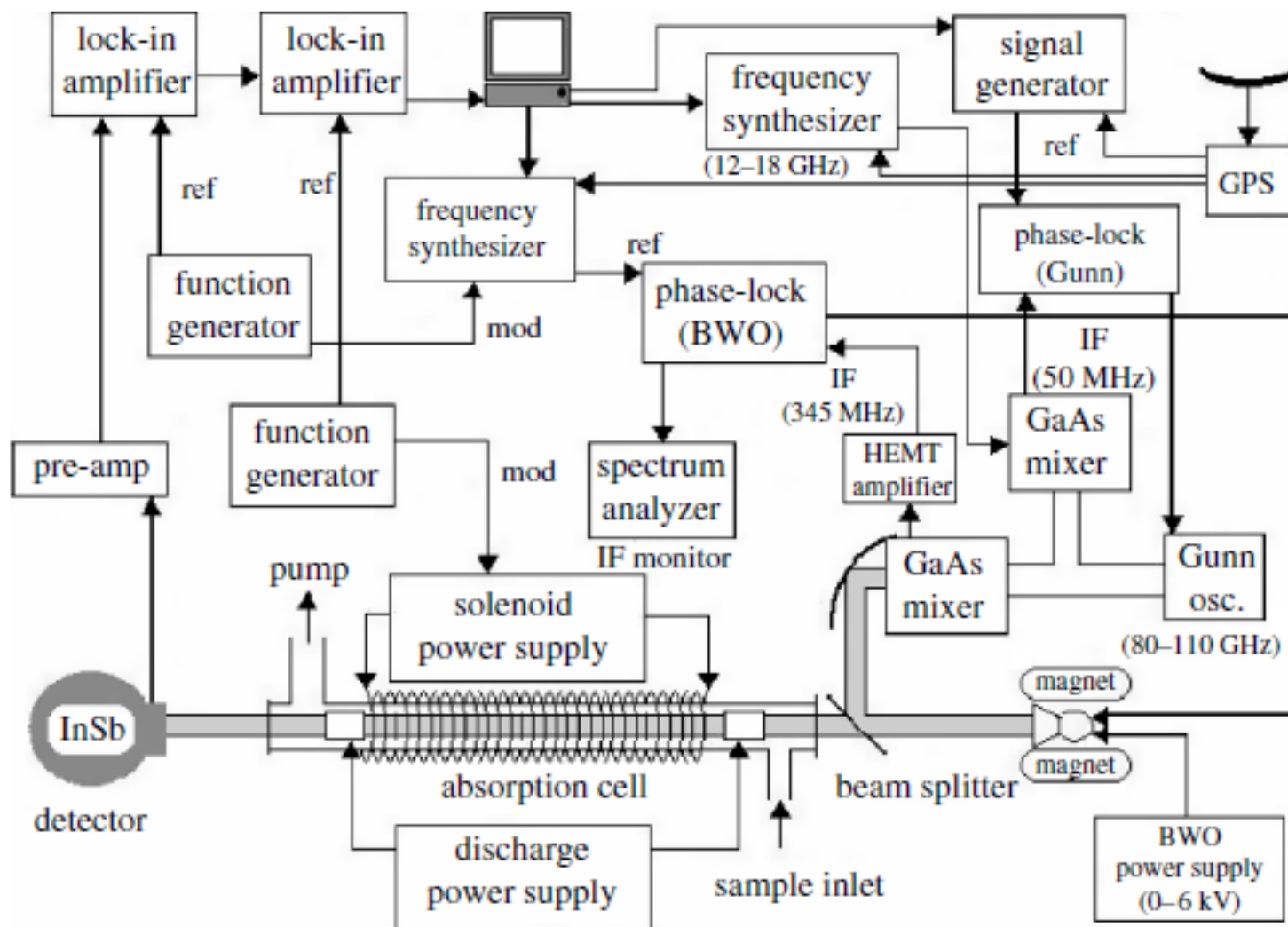
MW- Sub-mm Spectroscopy in Japan

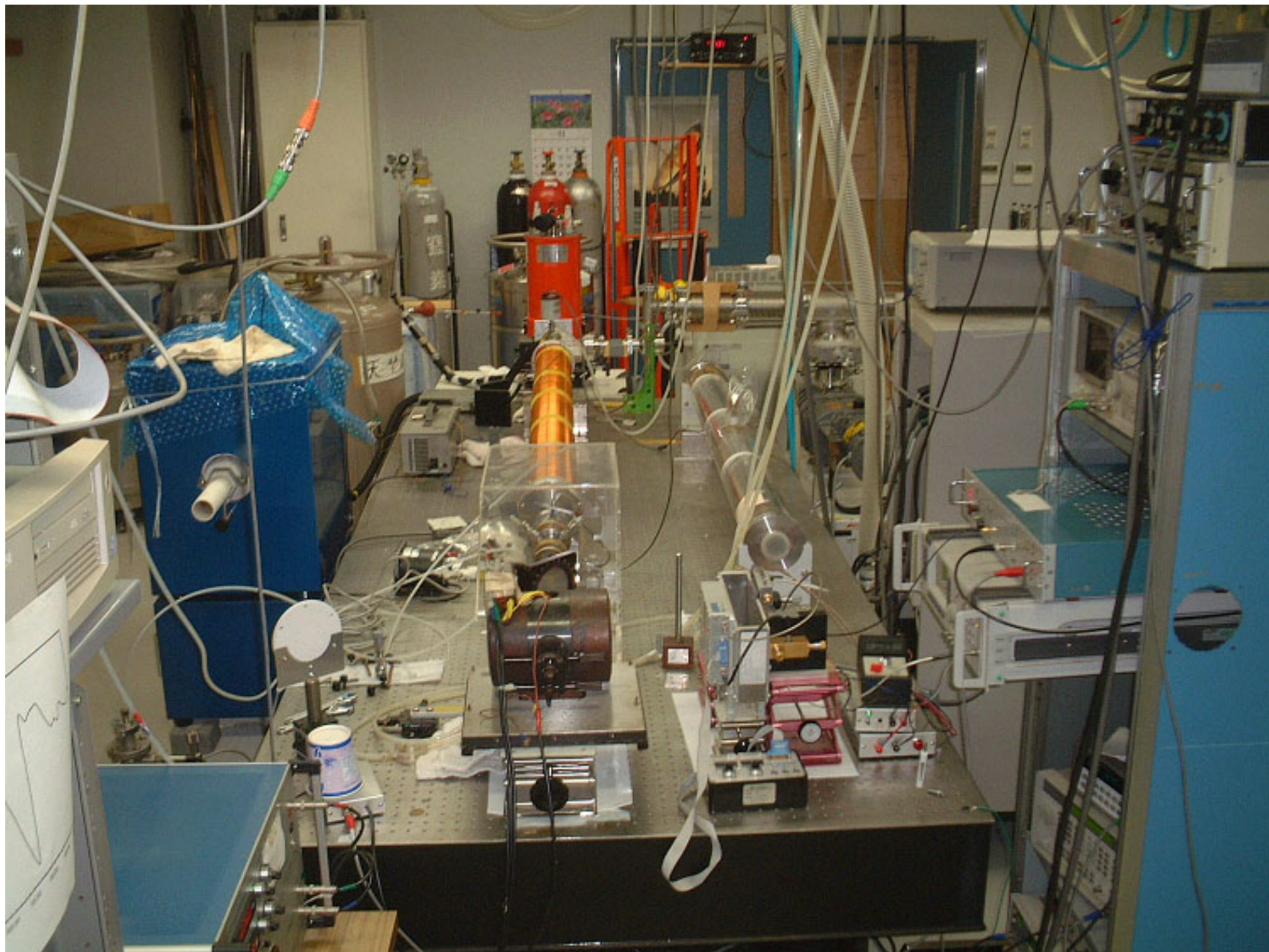
- Fukui U. (S. Saito)
- Kanagawa Institute of Technology (Y. Kawashima)
- Kanazawa U. (M. Fujitake)
- Kyushu U. (K. Tanaka)
- Okayama U. (K. Kawaguchi)
- Shizuoka U. (T. Okabayashi)
- Toho U. (H. Ozeki)
- Tokyo Institute of Technology (H. Kanamori)
- U. of Tokyo (Y. Endo)
- U. of Toyama (F. Matsushima)

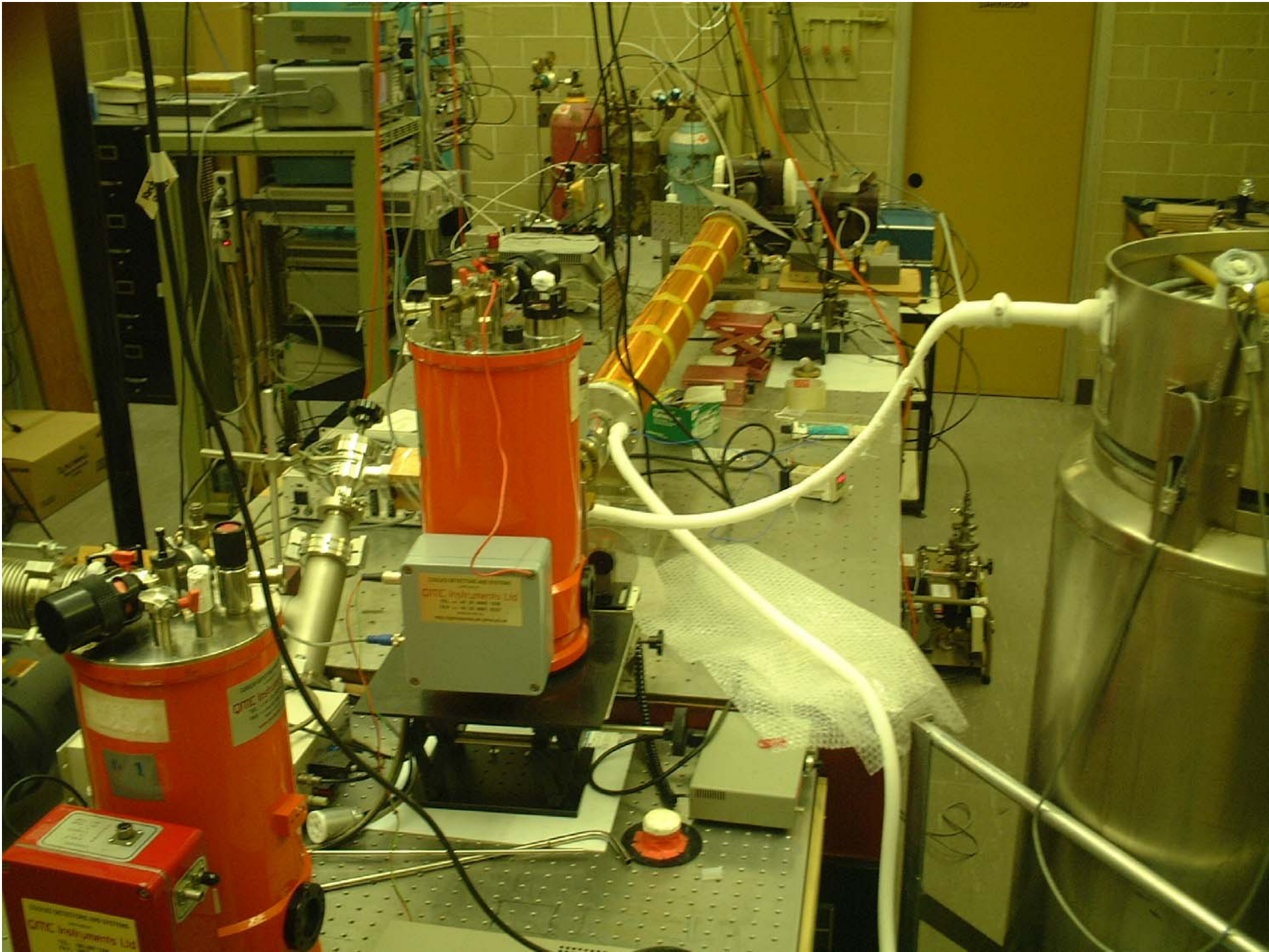
- Ibaraki U. (T. Amano) \longrightarrow Waterloo

- TuFIR ~several THz (Toyama)
- BWO ~860 GHz (Kanazawa, Kyushu, Tokyo
Inst. Tech)
- Multiplier ~1.5 THz (Toho)
~830 GHz (Fukui)
~360 GHz (Okayama, Shizuoka)
~200 GHz (Toyama)
- Emission Spectroscopy ~650 GHz (Toho, JAXA)
- FTMW ~50 GHz (Shizuoka)
~40 GHz (Tokyo)
~26 GHz (Kanagawa Inst. Tech)

Sub-mm Spectrometer at Waterloo



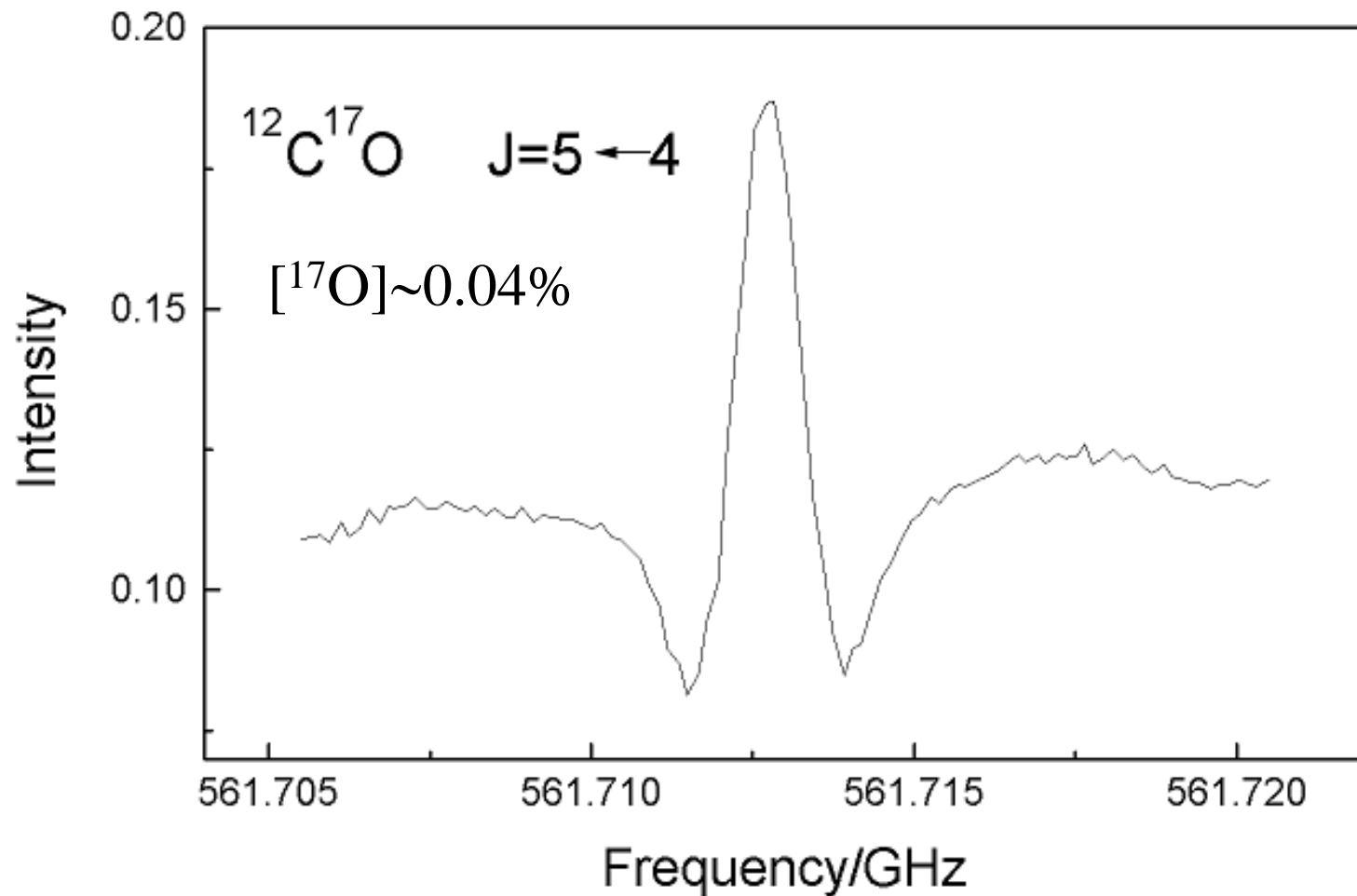


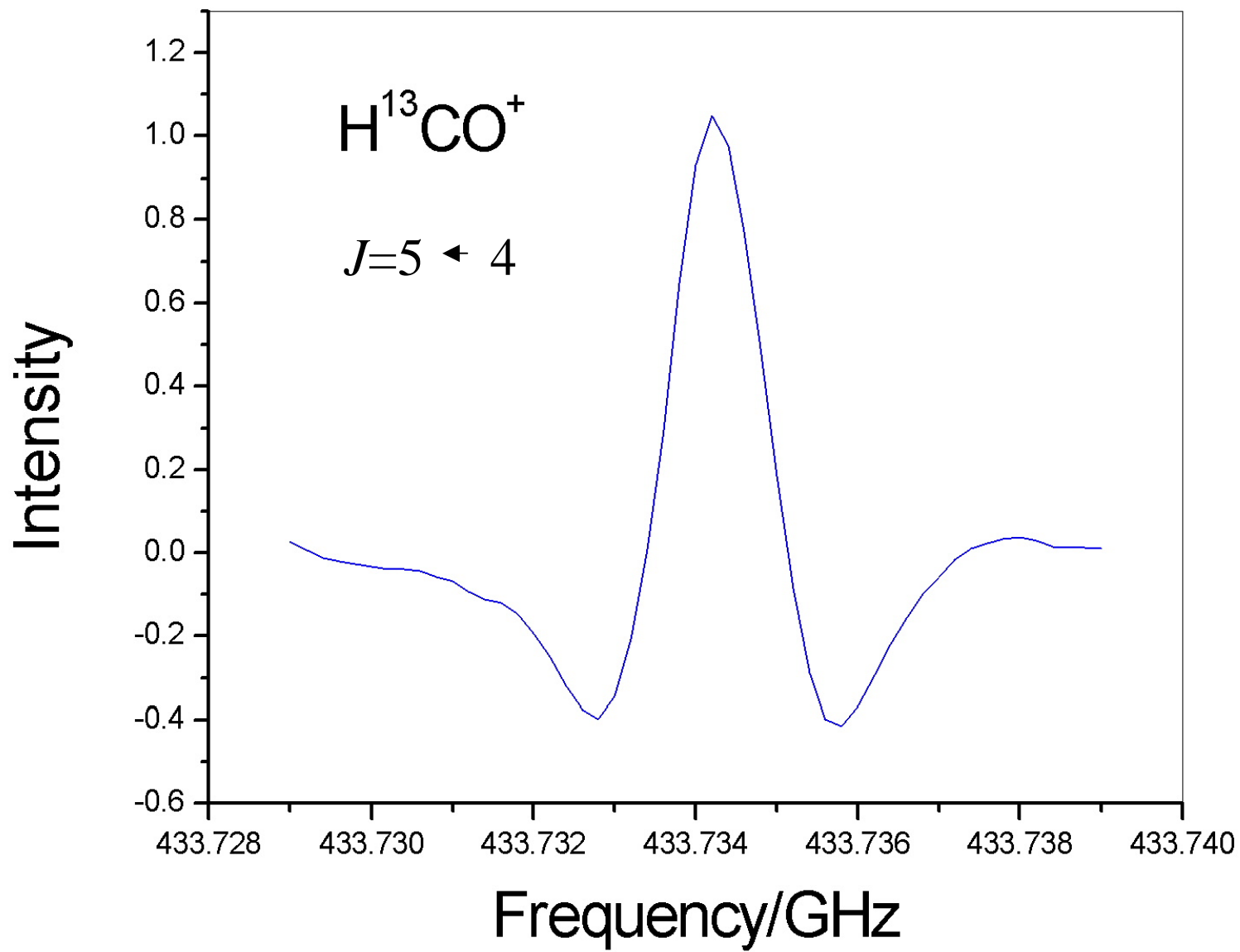


Sensitivity of the spectrometer

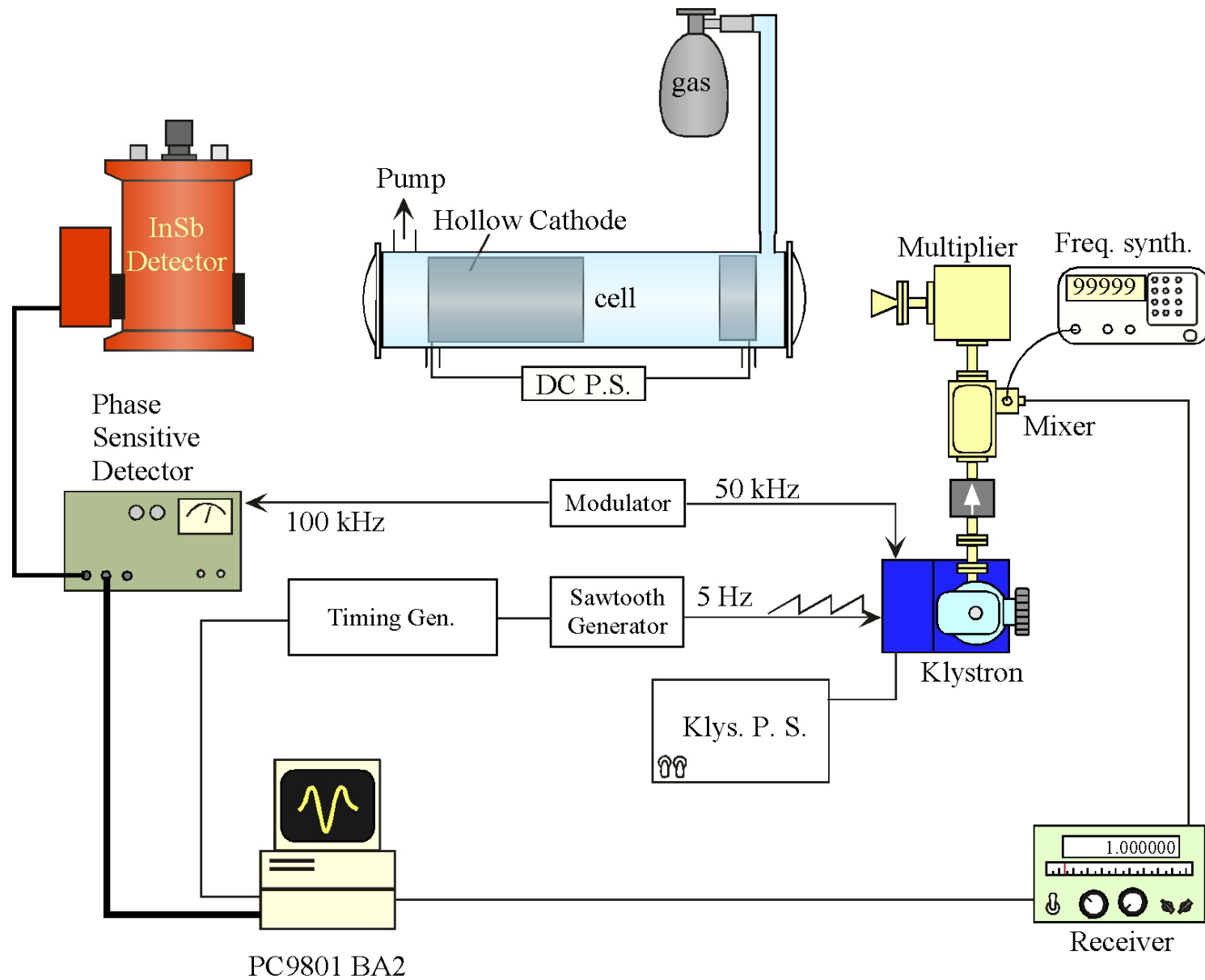
$$I = I_0 e^{-\tau} \quad \frac{\Delta I}{I_0} = \frac{I_0 - I}{I_0} = 1 - e^{-\tau} \approx \tau \quad \tau_{\min} \approx 3.1 \times 10^{-6}$$

(1sec integration time)



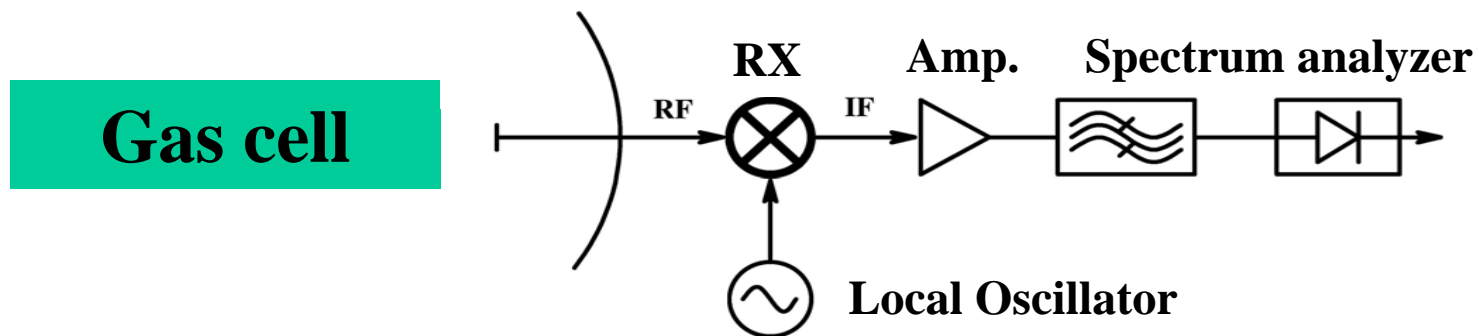


High Sensitivity Submillimeter-Wave Spectrometer, Fukui Univ. (~830 GHz)



Emission Spectrometer

Japan Aerospace Exploration Agency (JAXA)



Frequency coverage: 610 - 660 GHz
(Can be expanded by replacing local oscillator)

FuFIR system at Toyama

Protonated rare gas atom
(molecular cation)

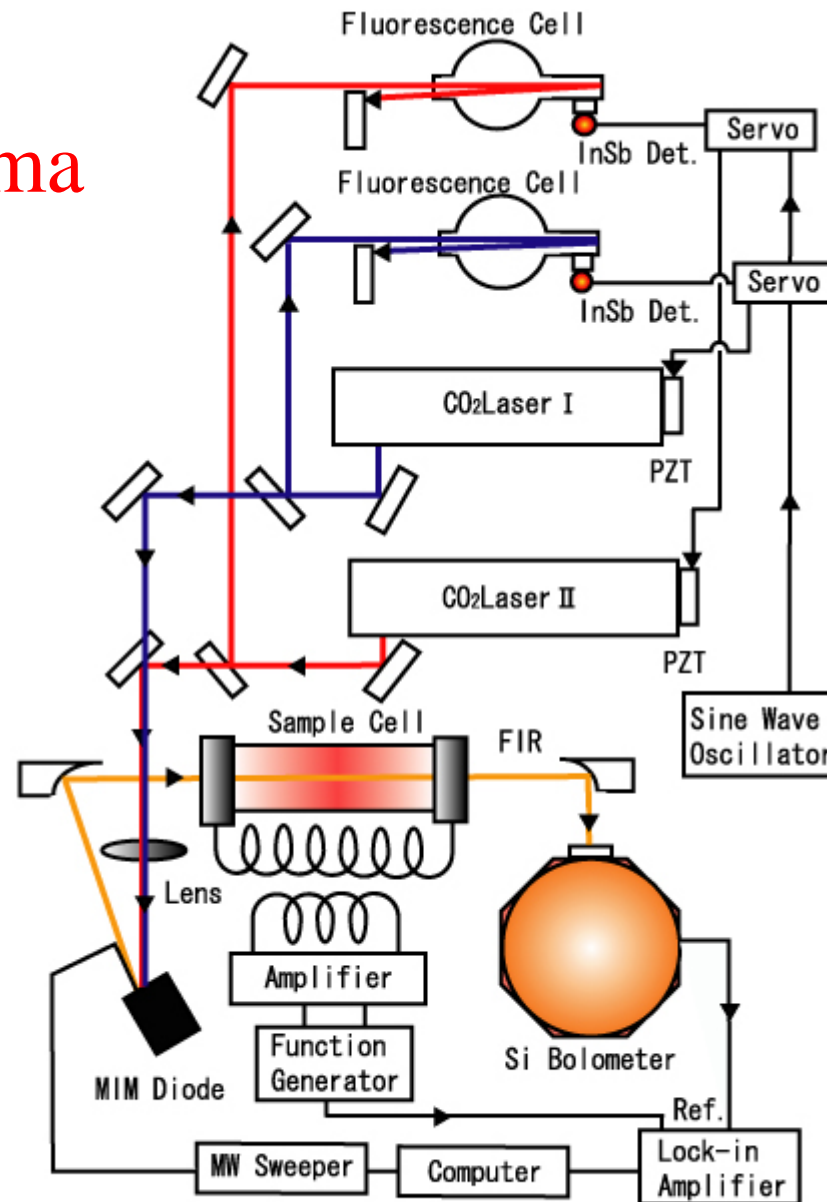


Fig.1 Experimental Setup of TuFIR spectrometer

Specs of TuFIR spectrometer

Frequency range:

DC ~ 5.2 THz (normal CO₂ laser)

~6.2 THz (isotope CO₂ laser, sequence band)

~10 THz (combination with other gas lasers)

Accuracy : about 30 kHz

(assuming 25 kHz for each laser)

Source power: 10⁻⁸ ~ 10⁻⁶ W

Molecules, radicals, and ions investigated with TuFIR in Toyama

(1) Rotational spectra of molecules and radicals

LiH, KH, ^{18}OH , NH, N^{18}O

H_2O (including isotopes, vibrationally excited states)

(2) Torsion rotation transitions of molecules with internal rotation

CH_3OH

(3) Rotational spectra of protonated rare gas atoms (+ ions)

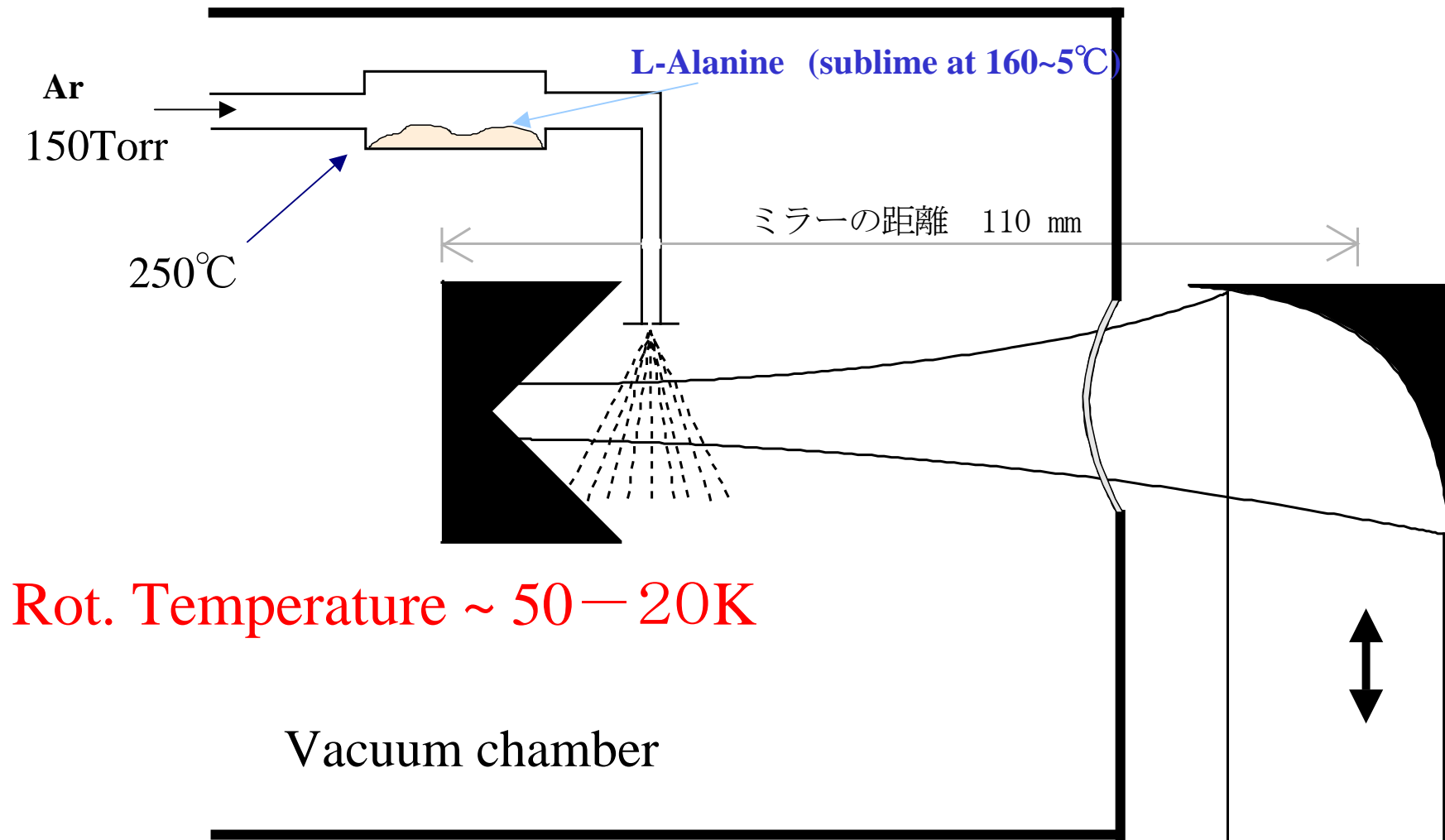
HeH^+ , NeH^+ , ArH^+ , KrH^+ , XeH^+ , H_2D^+

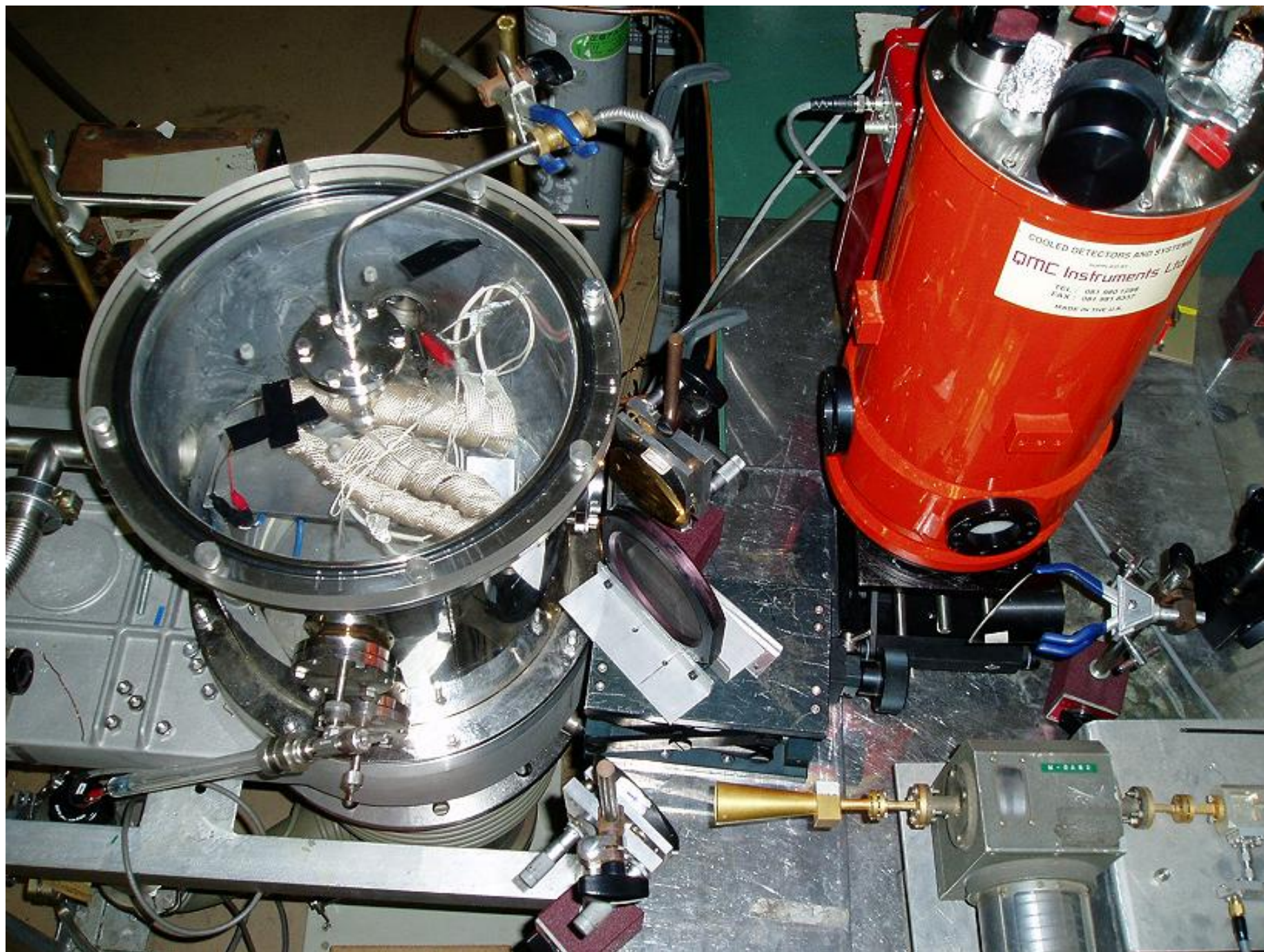
(including isotopes of rare gas atoms and H)

(4) Rotational spectra of molecular anions

OH^- , OD^-

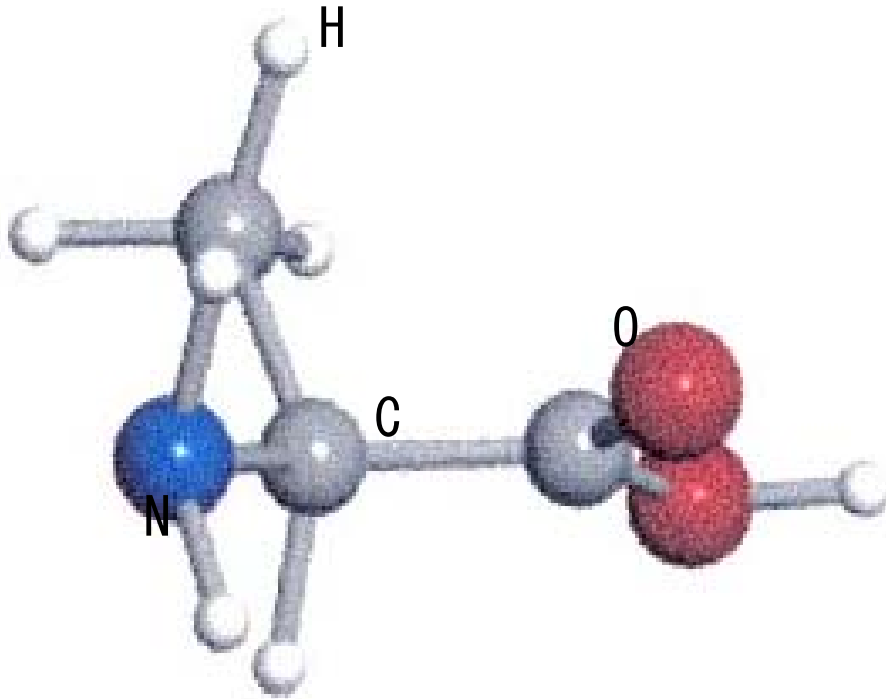
Experimental Setup (Okayama)



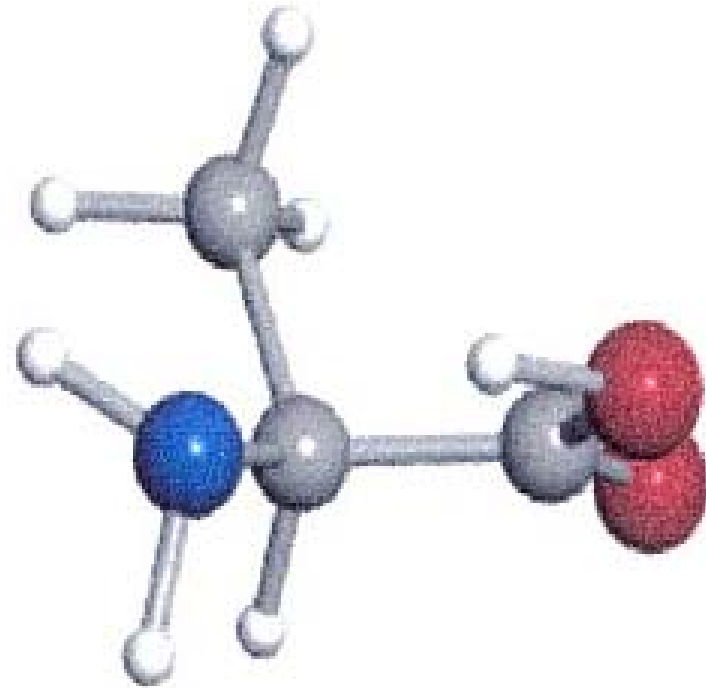


α -Alanine

simplest amino acid with optical isomers



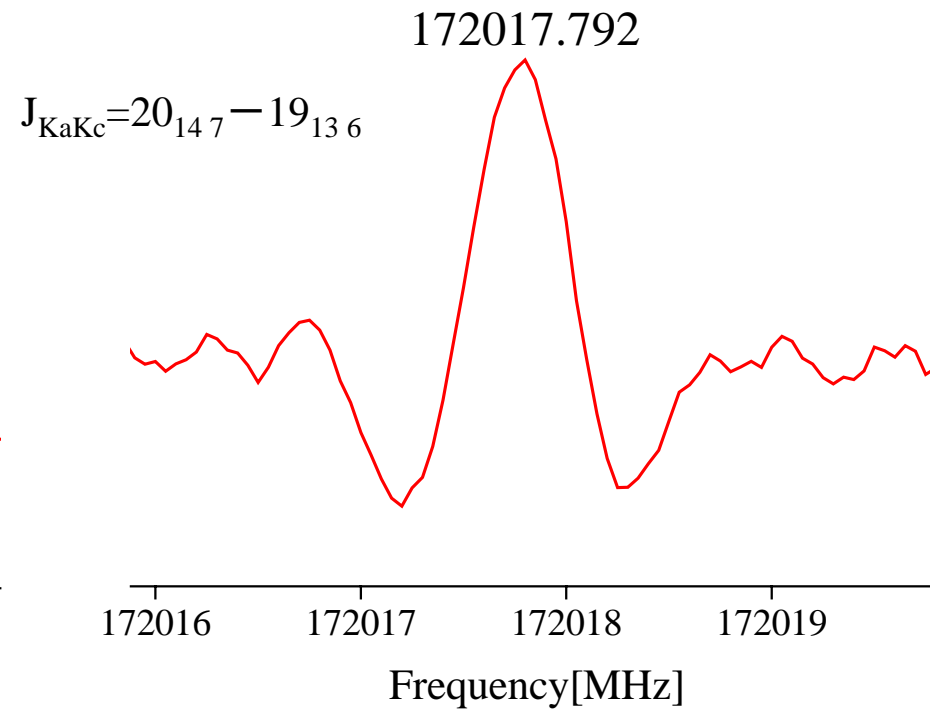
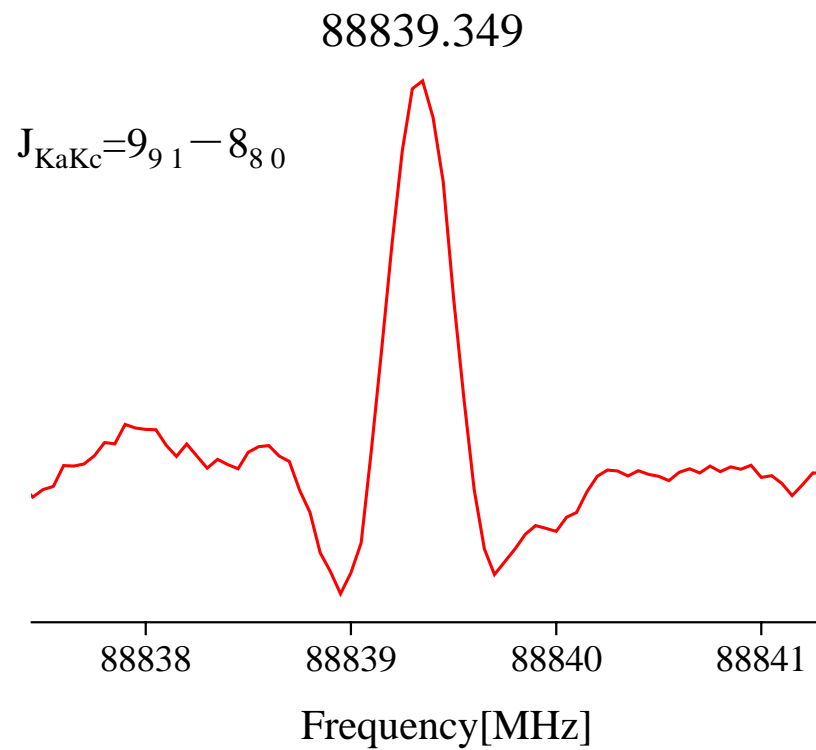
Conformer I



Conformer II

Data available below 71 GHz
Extended to higher frequency

Laboratory lines of alanine



Dynamical Structure of Peptide Molecules

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ABSTRACT

In view of the importance of the peptide linkage in structural biology, we have carried out intensive investigations on peptide molecules consisting of a peptide linkage with one or two substituents in the gas phase by Fourier transform microwave spectroscopy, paying special attention to the internal rotation of the substituents relative to the central linkage framework. We have found that, in sharp contrast with the stiff structure around the central C–N bond of the linkage, the internal rotations of the substituents are of low frequency and thus of large amplitude and are extremely susceptible to their local environment such as the presence of other substituents.

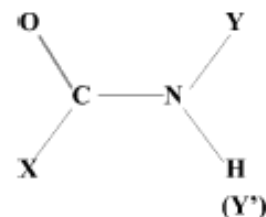


FIGURE 1. Peptide molecule.

spectroscopy. When our results are combined with results previously reported by other groups, we are able to derive characteristic features of the linkage system, which can be of considerable significance to structural problems in biology. Our results will be also of great interest from the viewpoint of molecular science, because the dynamical structure of the peptide linkage system is quite unique, much different in character from that of most other organic molecules.

To start with, we decided to focus our attention on the internal rotation of substituents X and Y directly bonded to the peptide linkage, because rotations about the C–X and N–Y bonds correspond to changes in the Ramachandran angles ψ and φ , respectively. We have also considered substitutions at the Y' position, although such substitutions only occur in natural peptides containing

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Toyama University Molecular Spectroscopy Atlas

Vol. 1 Methanol CH_3OH

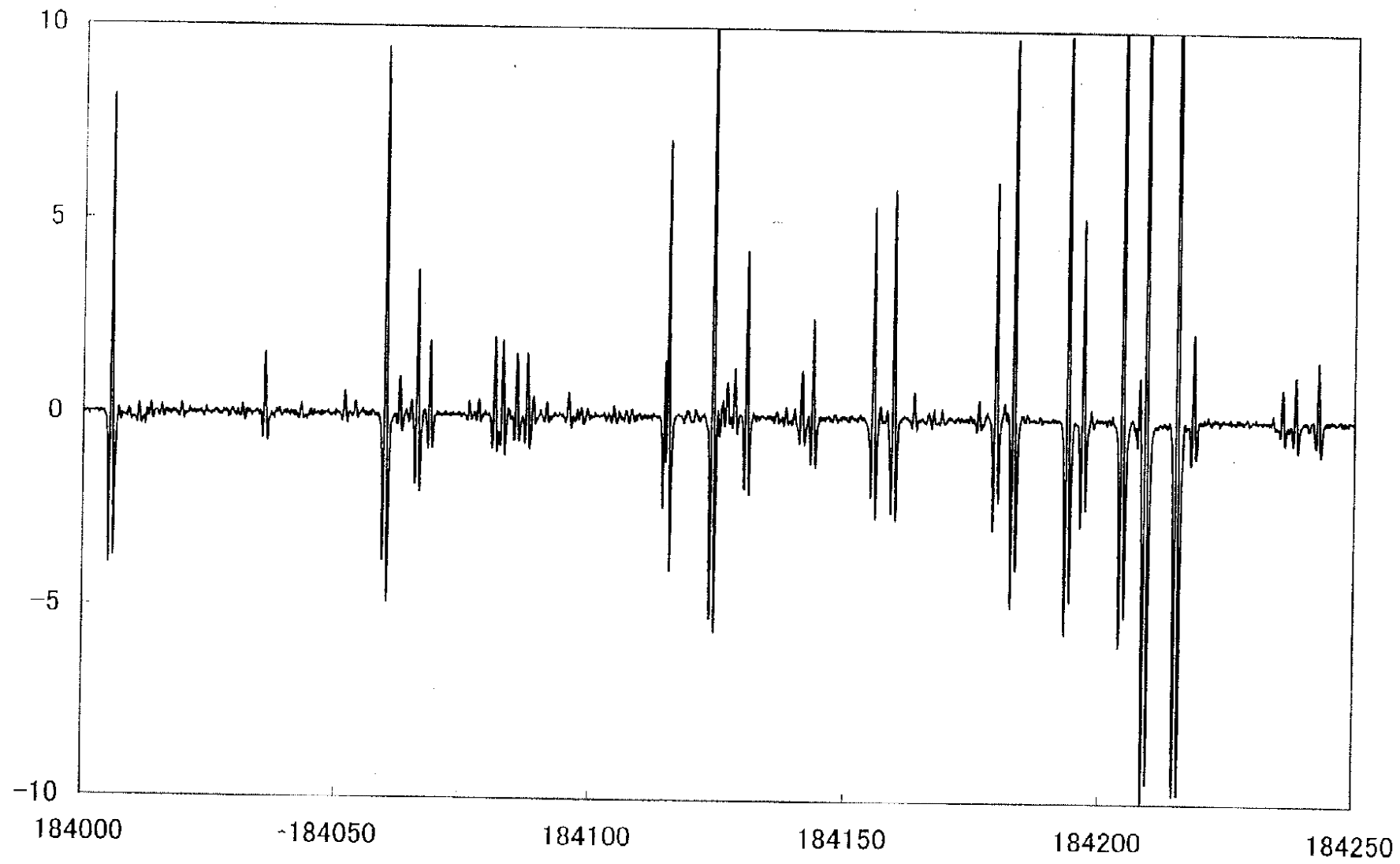
Vol. 2 Acetamide CH_3CONH_2

Vol. 3 Methyl formate HCOOCH_3

Vol. 4 Ethyl methyl ether $\text{C}_2\text{H}_5\text{OCH}_3$

18~200 GHz

(to be extended up to 340 GHz)



Frequency/MHz

Future direction?

Funding

- ALMA-J **not promising**
- JSPS (Japan Society for Promotion of Science)

Lack of man power

