Development of a Stark velocity filter for studying cold ion-polar molecule reactions

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Background and Motivation

1. Ion-polar molecule reactions play important roles in synthesis of interstellar molecules
   → It is necessary to understand ion-polar neutral systems, before more definitive conclusions can be reached for chemical evolution in dark interstellar clouds usin "UMIST" data base (Wakelam et al. A&A 2006)

2. There are only a small number of experimental reaction-rate constants measured at low temperatures.
   → Benchmark data to test the scaling formula of the capture rate in ion-polar molecule collisions and other quantum chemical calculations

Capture rate by "trajectory scaling approach" based on classical trajectory technique※

$$k_{cap} = 2\pi e[0.62 + 0.4767x]\sqrt{\alpha/\mu}, \quad x \equiv \mu_D / \sqrt{2\alpha k_B T} \geq 2$$

(α: polarizability, μ: dipole moment, T: temperature, k_B: Boltzmann constant)

※T. Su & W. J. Chesnavich, JCP1982

Previous studies

- T. Baba *et al.* " Chemical reaction between sympathetically cooled molecular ions and NH_3 : $H_3O^+ + NH_3 \rightarrow NH_4^+ + H_2O$ " (JCP 2002)

- G. Rempe *et al.* " First demonstration of Stark velocity filter to produce slow polar molecules " (PRA 2004)

- T. P Softley *et al.* " Reaction rate measurement between Ca^+ Coulomb crystal and cold CH_3F " (PRL 2008)

- S. Willitsch *et al.*, " Preliminary reaction rate measurement between slow ND_3 and sympathetically cooled OCS^+ ions " (Faraday Discuss. 2009)

We are now developing a new apparatus composed of a Stark velocity filter and cryogenic linear ion trap.

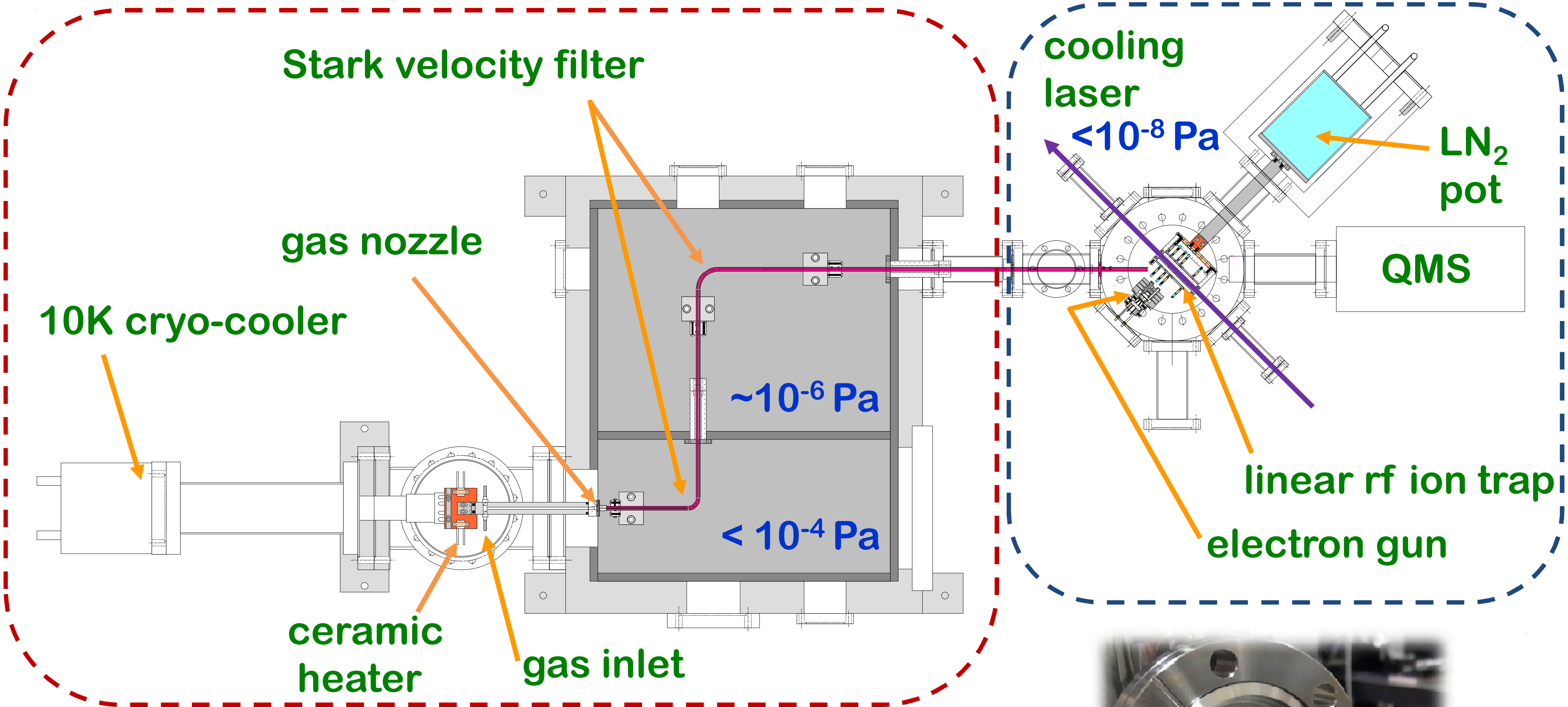
Extension in this study

1. Many kinds of cold molecular ions will be supplied by sympathetic laser cooling → CaH^+, CaF^+, N_2^+, CH_2O^+, ND_3^+ …

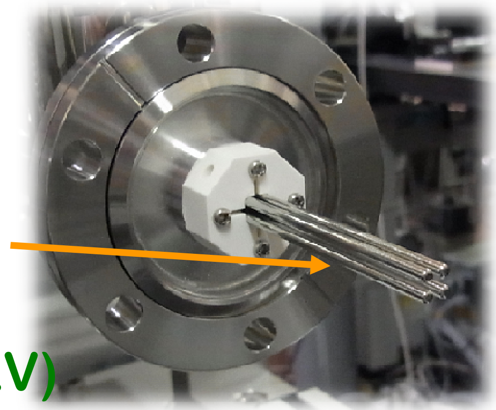
2. Many kinds of slow polar molecules will be supplied.

formula	name	μ [D]	formula	name	μ [D]
NH_3	ammonia	1.468(c)	CH_3NO_2	nitromethane	3.46
ND_3	deuterated ammonia	1.5(c)	$C_6H_5NO_2$※	nitrobenzene	4.21
CH_2O	formaldehyde	2.34(a)	C_2H_5OH	ethanol	1.69
CD_2O※	deuterated formaldehyde	2.34(a)	CH_3OH	methanol	1.66
H_2O	water	1.82(a)	CH_3COCH_3	acetone	2.9
D_2O	deuterium oxide	1.85(a)	CH_2F_2	difluoromethane (freon 41)	1.96(b)
HDO	deuterium protium oxide	0.66(a) 1.73(b)	CH_3F	fluoromethane (freon 23)	1.86(a)
CH_3CN	acetonitrile methyl cyanide	3.92	CH_3CHO※	acetaldehyde	2.7

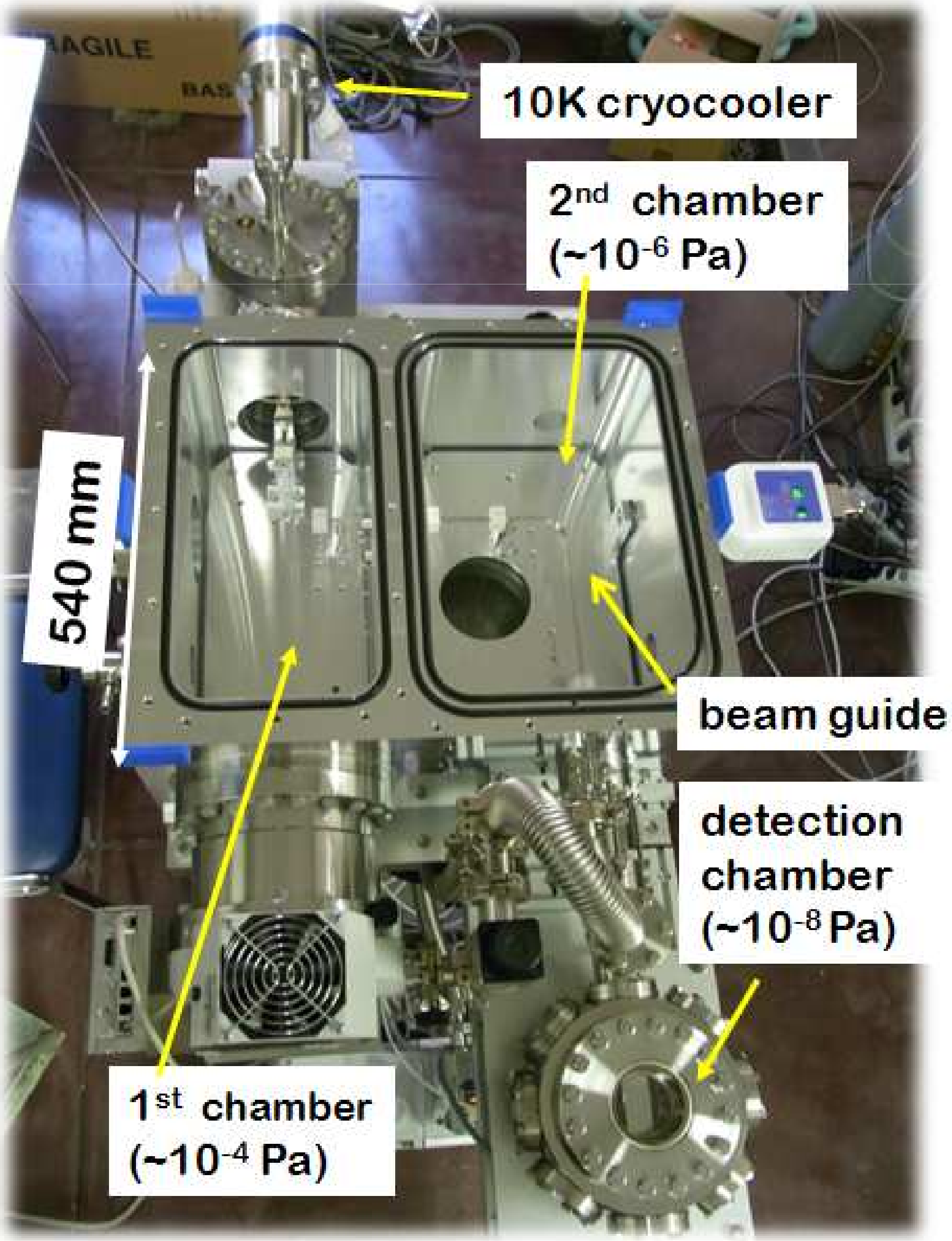
Overview of experimental setup

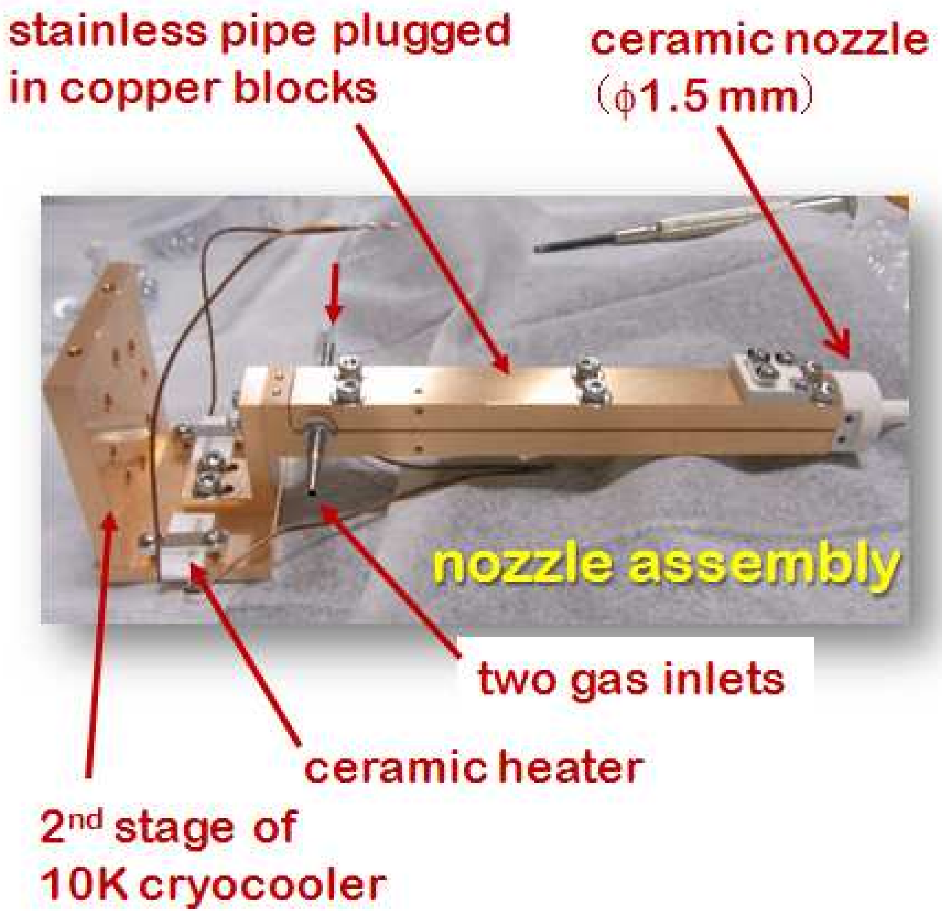


- ◆ Curveture radii of 1st and 2nd bent sections
  → R = 12.5 mm, 25.0 mm
- ◆ total length of the beam guide
  → L = 941.8 mm

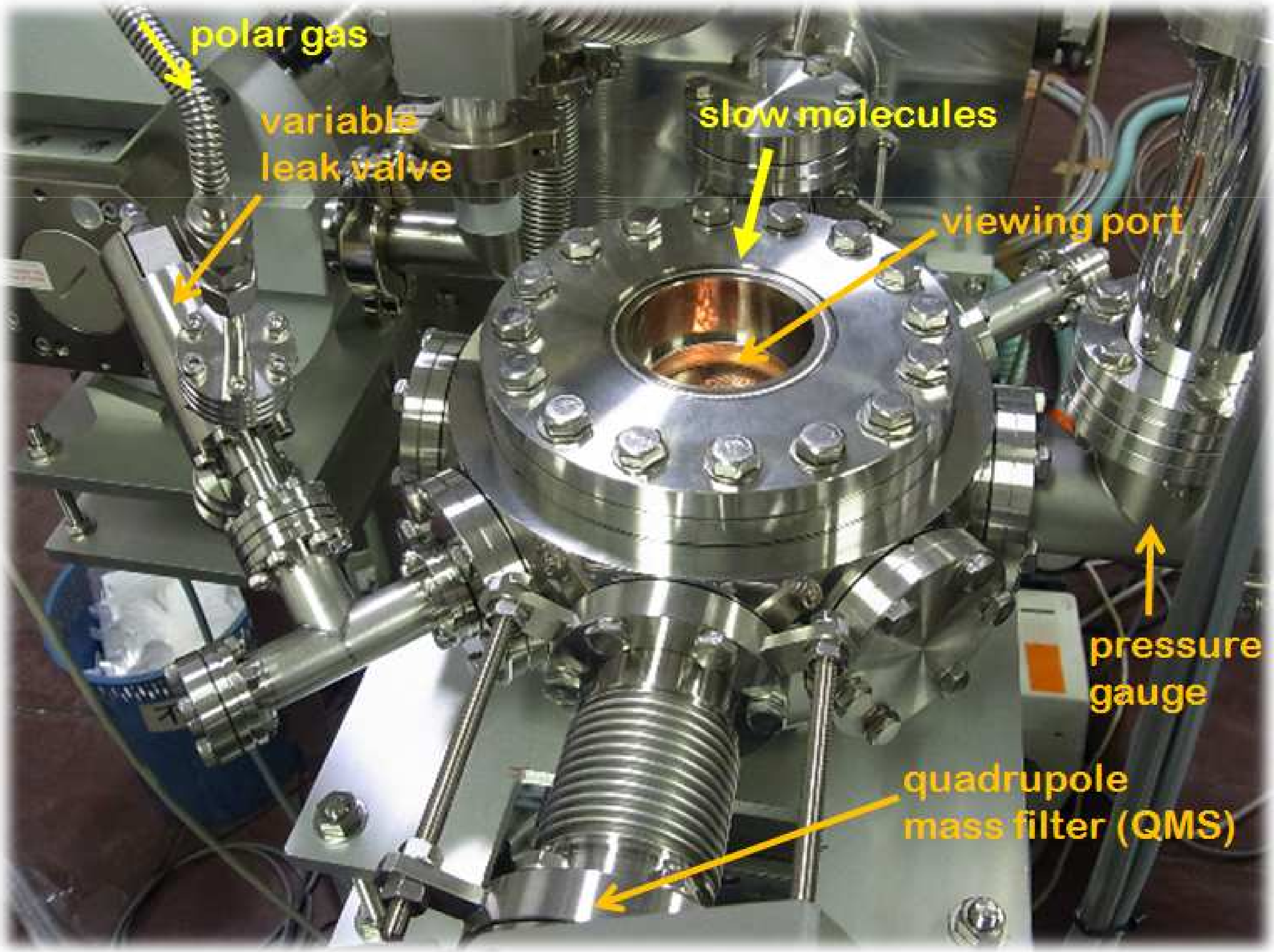


Stark velocity filter



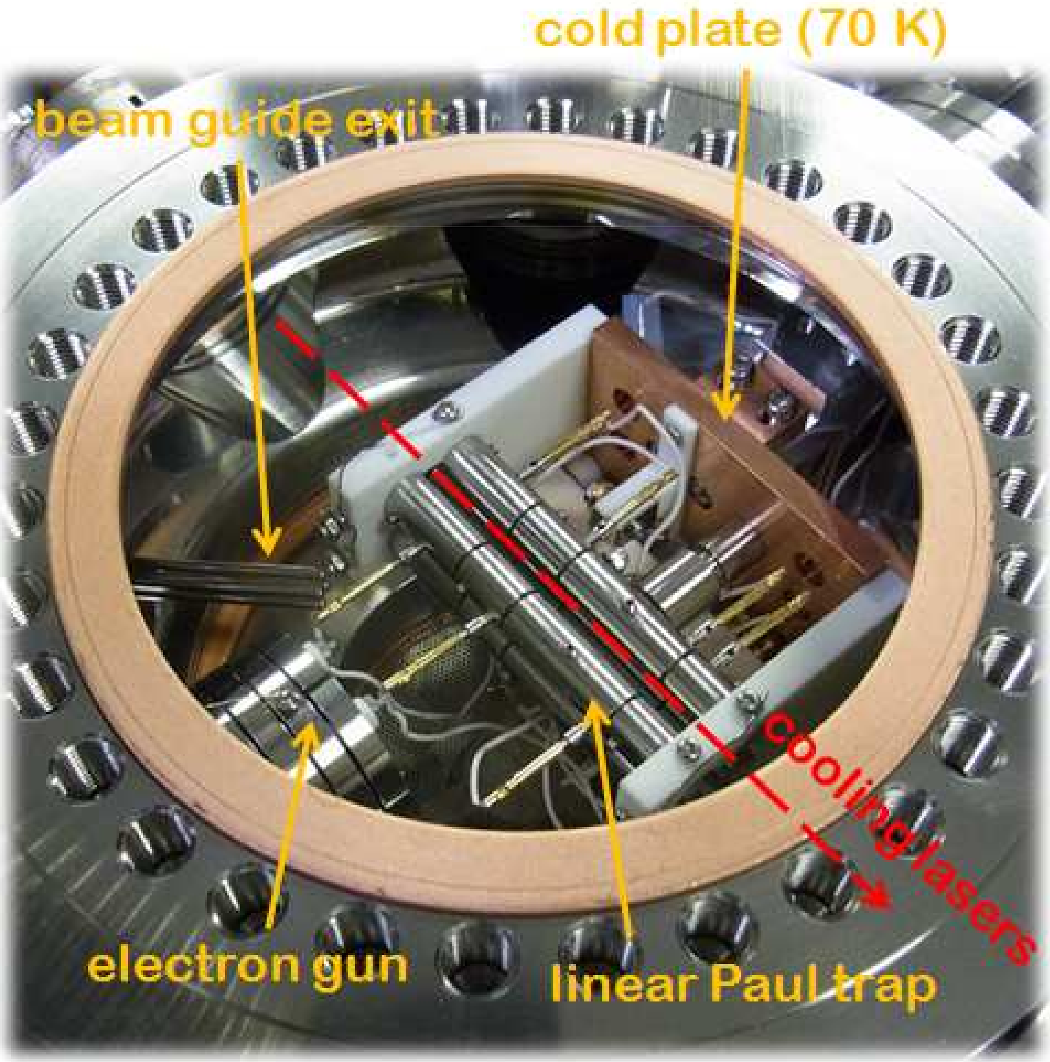


Detection vacuum chamber



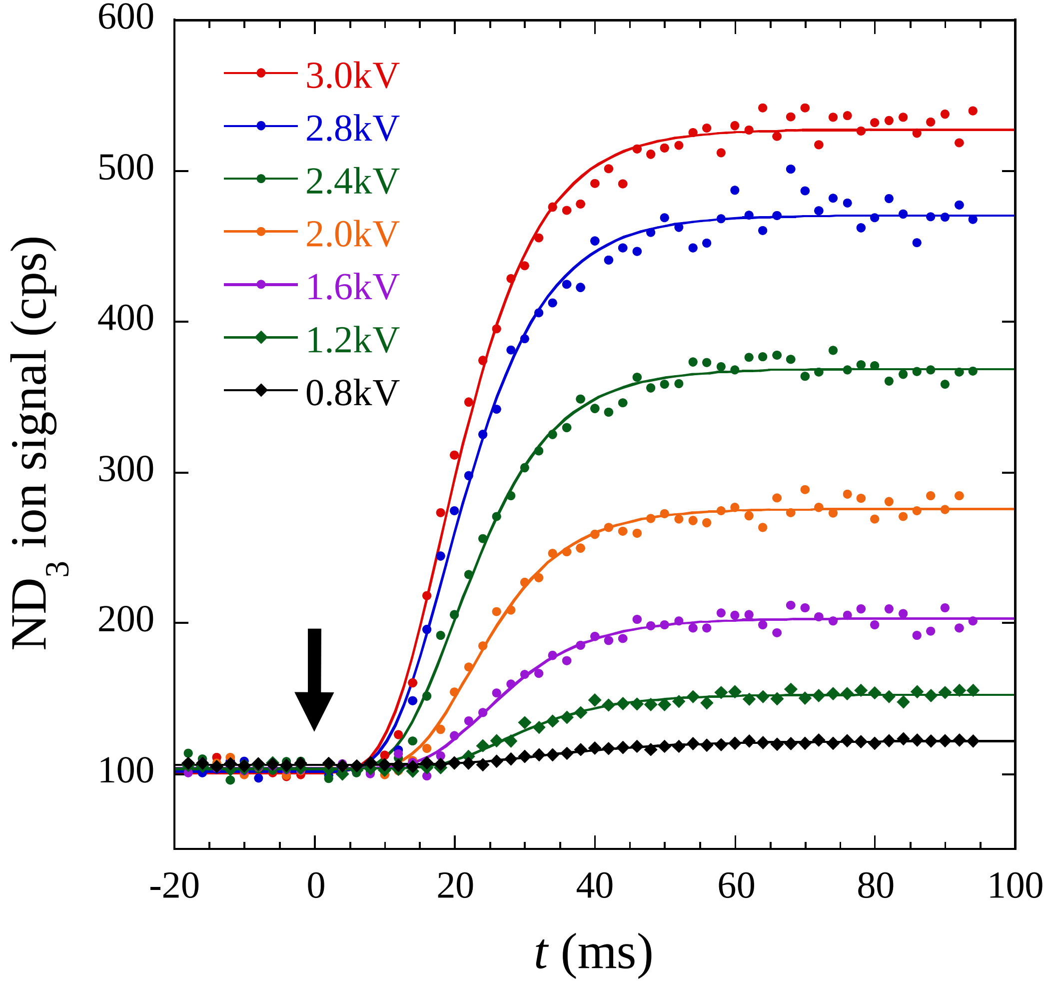
Linear Paul trap

overview of the detection chamber



Time-of-flight measurement of slow ND_3 molecules

ND_3@41±1mTorr, 295K



◆ Velocity distribution

$$f(v) = \frac{L}{v^2}\left(\frac{dI(t)}{dt}\right), \quad t = L/v$$

L: **flight distance**

◆ Gompeltz function

$$I(t) \propto \exp[-\exp[-k(t - t_c)]]$$

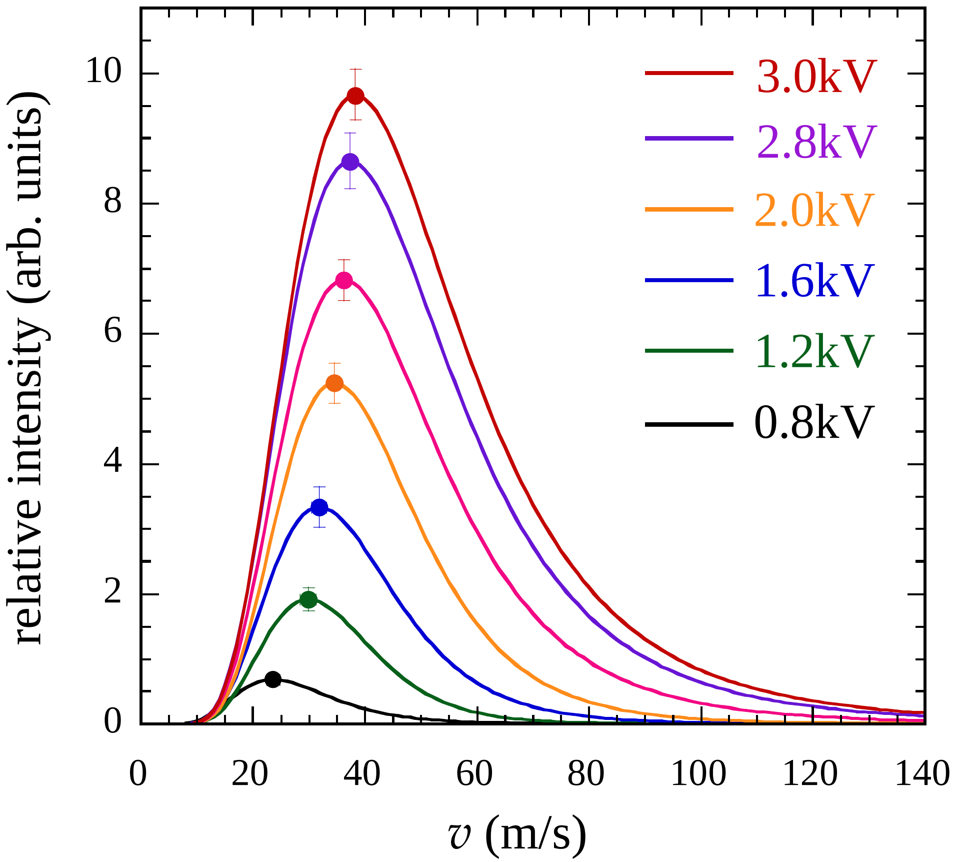
asymmetric growth curve

➡ **I(t) well reproduce TOF signal※**

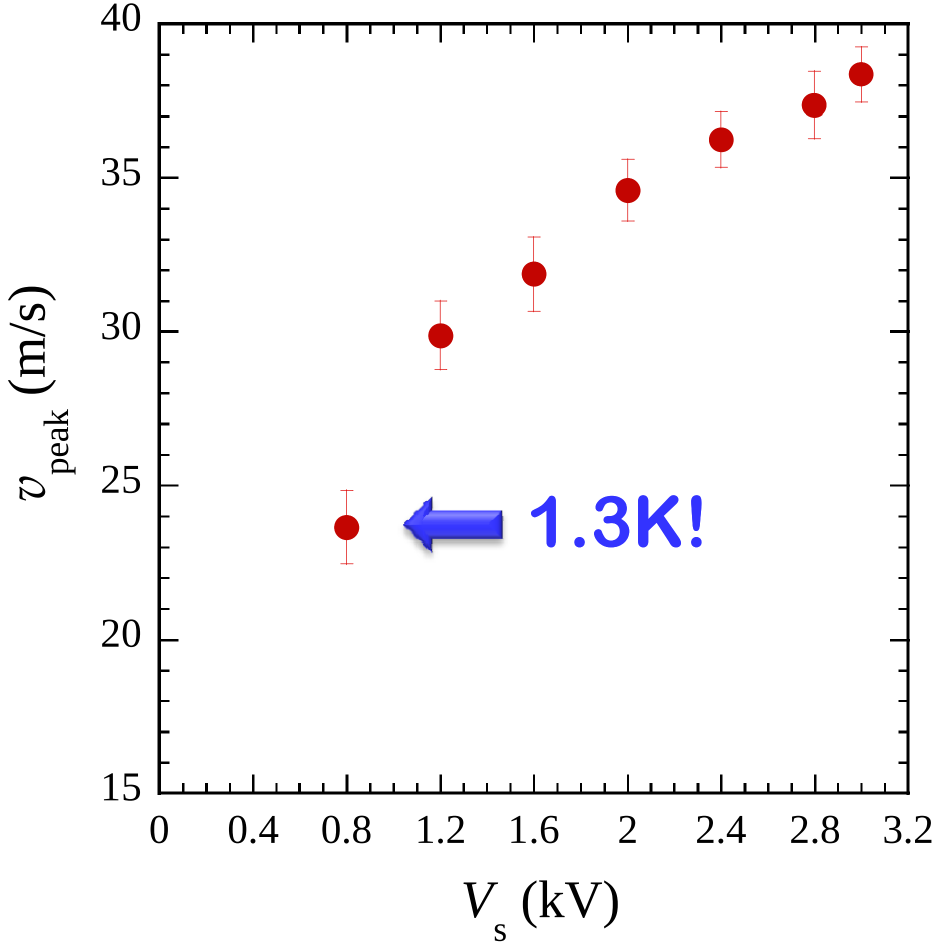
※M. T. Bell et al., Faraday Discuss.142, 73 (2009)

Velocity distribution

ND_3@41mTorr, 295K

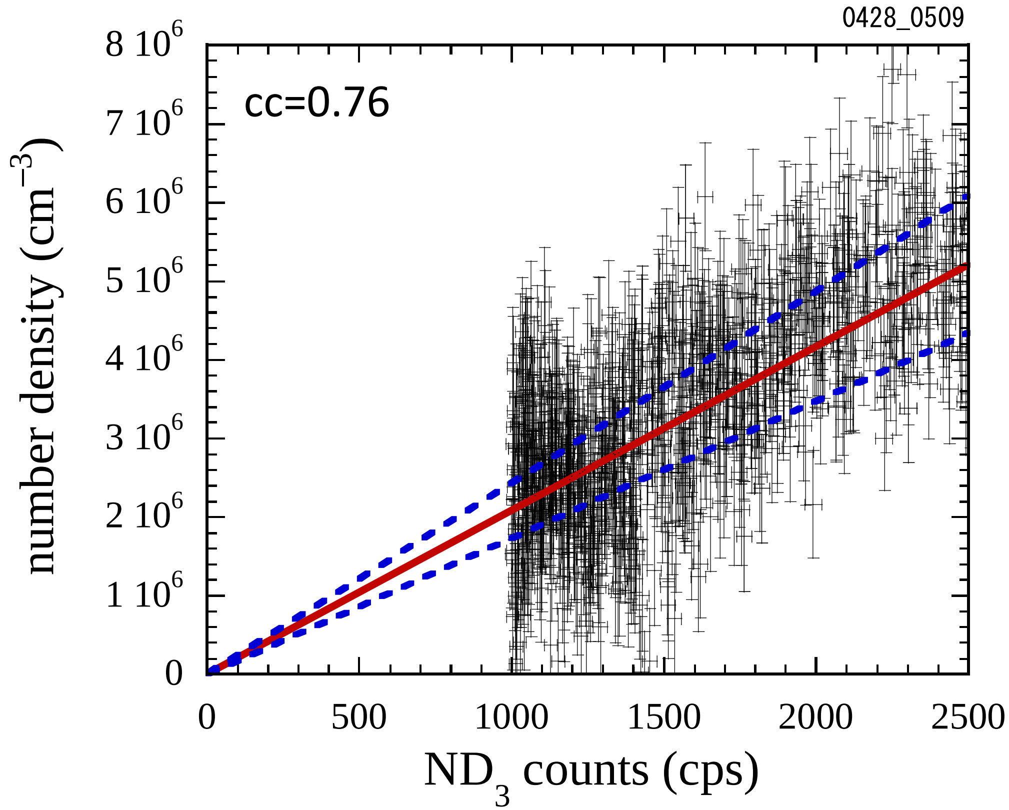


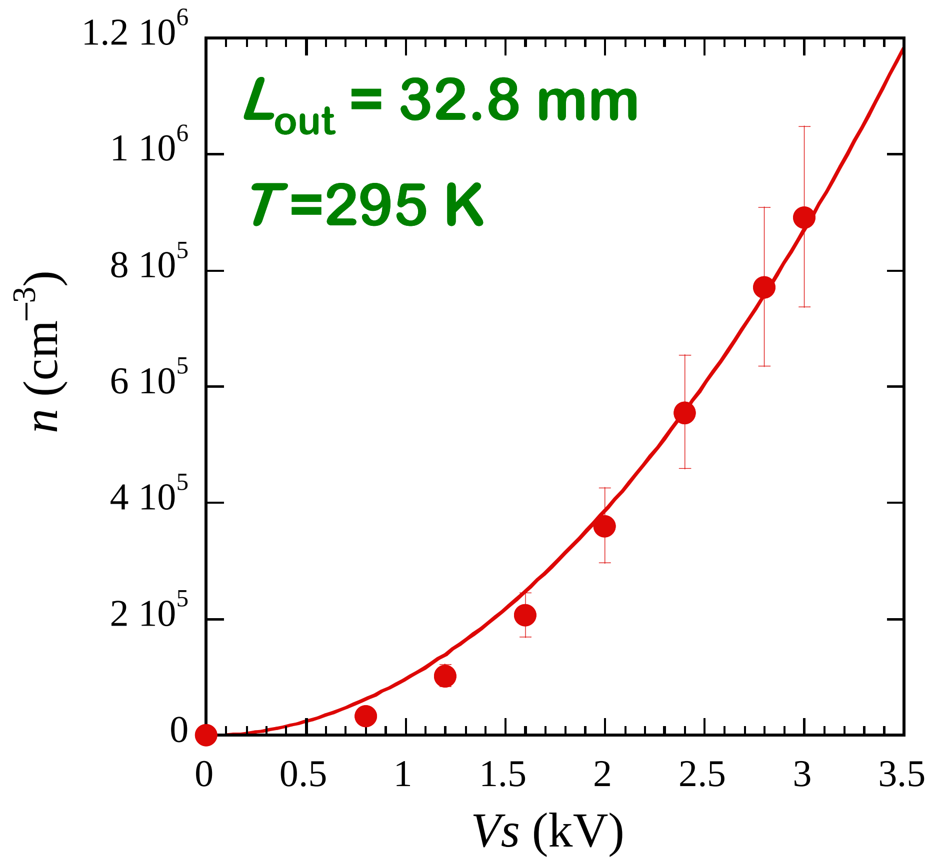
A plot of peak velocity



Number density of slow ND_3

ND_3 gas was intentionally leaked from the variable leak valve.



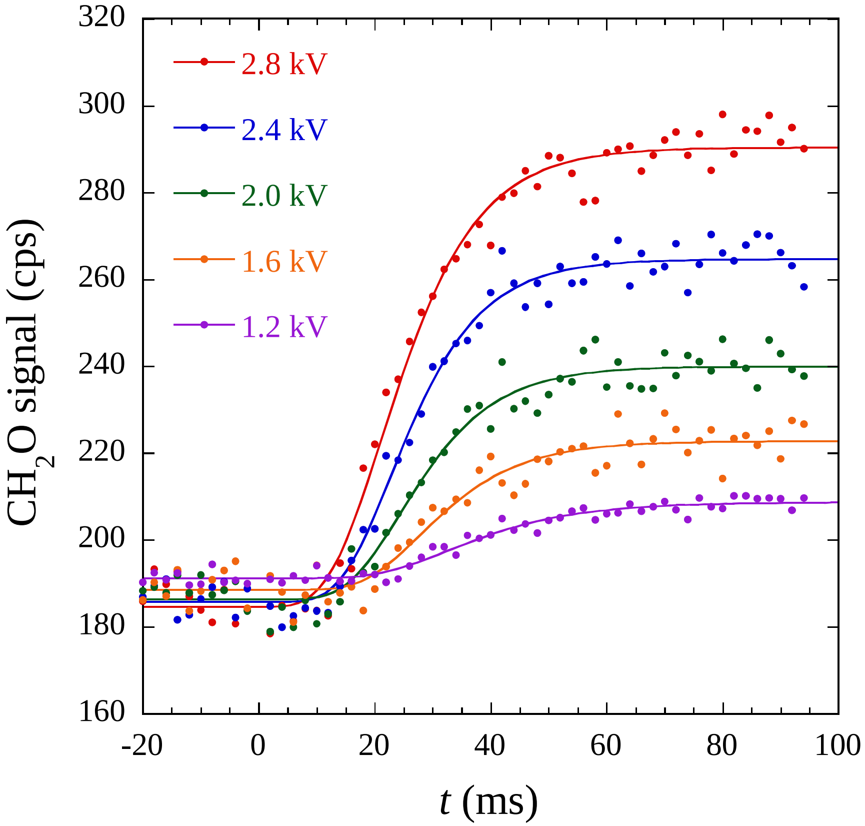


$$n = 2.1(3)\times 10^{3} I_{QMS}\,[\mathrm{cm}^{-3}]$$

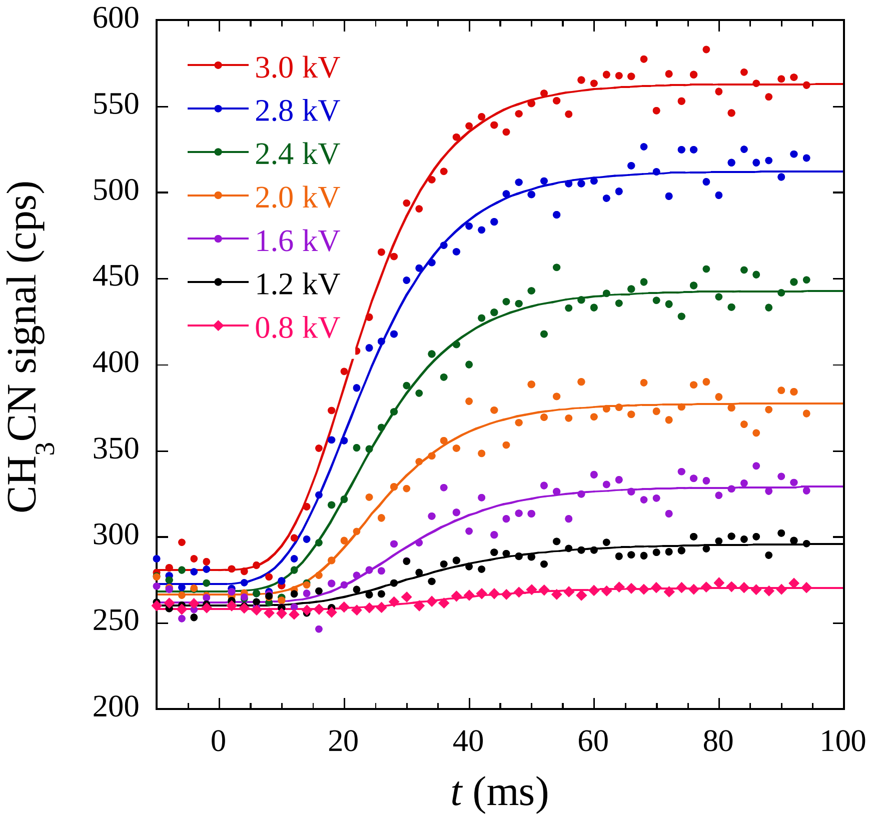
$$n_{\max} \approx 9\times 10^{5}\,[\mathrm{cm}^{-3}]\,@\,3\mathrm{kV}$$

TOF signals of CH_2O and CH_3CN

CH_2O @ 41±1mTorr, 295K



CH_3CN @ 32±1mTorr, 295K



The slowest peak velocity corresponds to a thermal energy of a few Kelvin.

Summary of production of slow polar molecules

nozzle temperature:295 K

molecule	M	v_{peak}(m/s)	T_{peak} (K)	n_{max}(cm^{-3})
ND_3	20.05	23 ~ 40	**1.3 ~ 3.8**	**9×10^5**
CH_2O	30.03	23 ~ 32	**1.9 ~ 3.7**	**1.3×10^6**
CH_3CN	41.05	23 ~ 34	**2.6 ~ 5.7**	**1.2×10^5**
NH_3	17.03	36.5	**2.7**	**2×10^5**

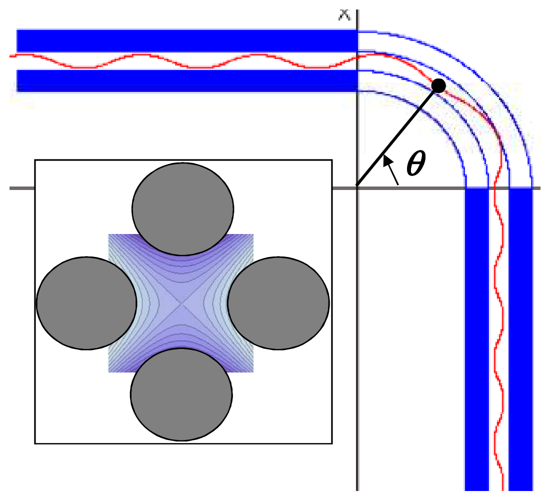
Cold ion-polar molecule reactions: $k = 10^{-8} \sim 10^{-9}$ (cm^3/s)

➡ Expected reaction-rate : $10^{-2} \sim 10^{-3}$ /s

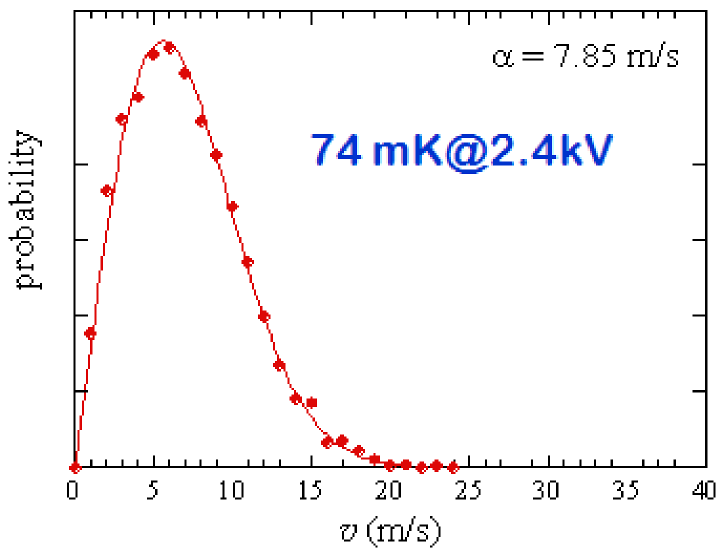
Simulation of Stark velocity filter

- Information of the transverse velocity distribution and the actual "cut-off" velocity
- Rotational state distribution of guided slow molecules
- Spatial dispersion of a slow molecular beam after passing through the beam guide (beam profile)

Trajectory of a slow ND_3



Transverse velocity distribution



Summary

- Stark velocity filter and cryogenic linear ion trap have been completed.
- Slow polar molecules (ND_3, NH_3, CH_2O, CH_3CN) with a thermal energy of a few Kelvin have been produced.
- Determination of the number density of the slow polar molecules has been conducted.
- Monte-Carlo simulation code has been developed for characterization of Stark velocity filter.