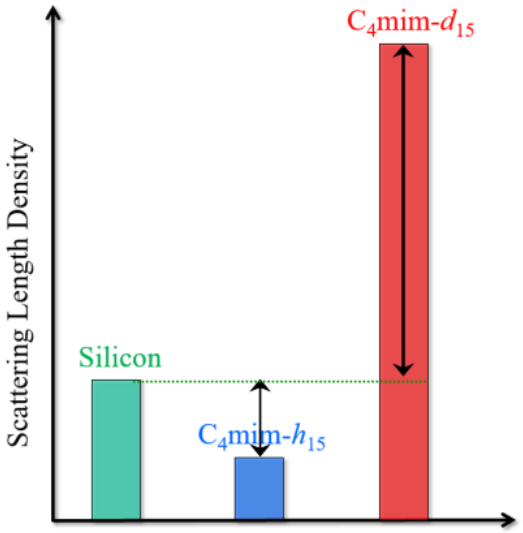
Chemical Deuteration Activities at CROSS

CROSS　Kazuhiro　AKUTSU

What is the purpose of deuteration?

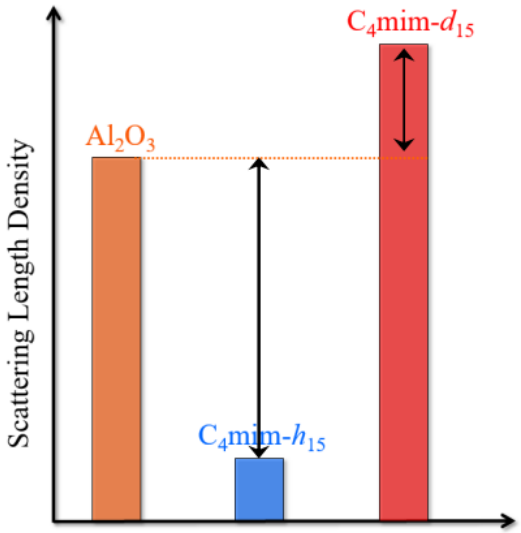
Neutron contrast

C_4mim-h_{15} < C_4mim-d_{15}



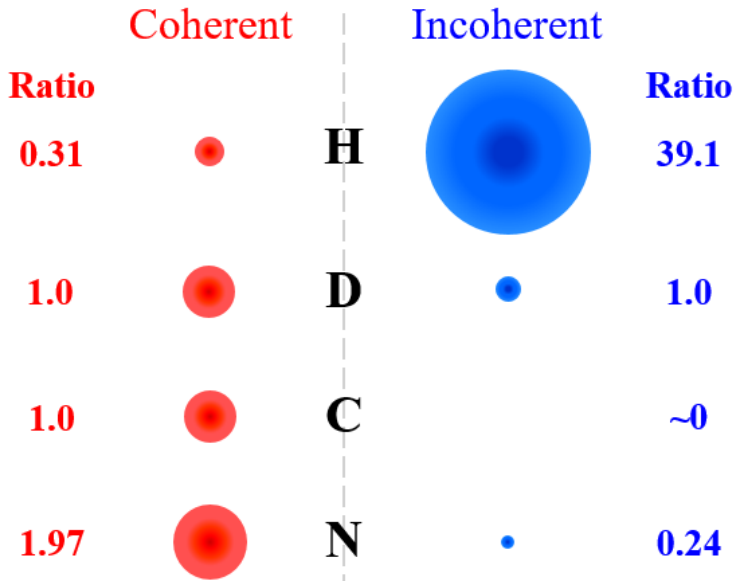
Neutron contrast

C_4mim-h_{15} > C_4mim-d_{15}



Incoherent scattering

C_4mim-h_{15} > C_4mim-d_{15}



For SANS or NR → contrast variation

For inelastic (quasi-elastic) neutron scattering

→ elimination of ^{1}H incoherent scattering

Use of deuterated materials @ J-PARC

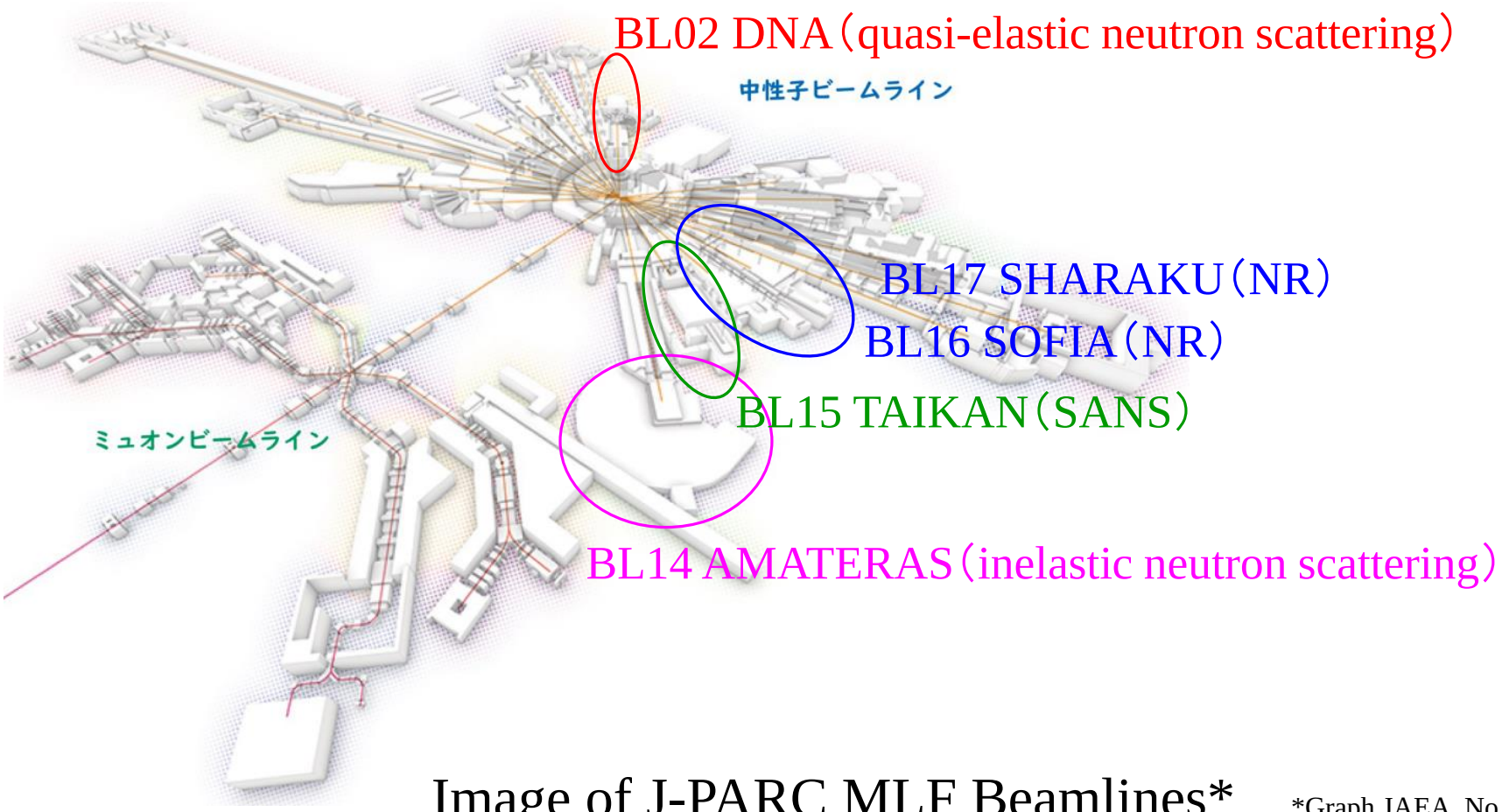


Image of J-PARC MLF Beamlines*

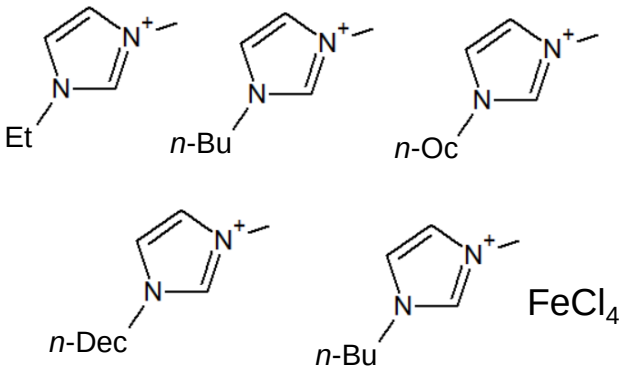
*Graph JAEA, No.11, 2019

Mary kinds of deuterated materials have been used at J-PARC MLF.

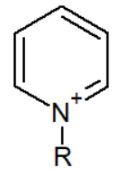
Deuteration Targets

Deuteration Requested Materials

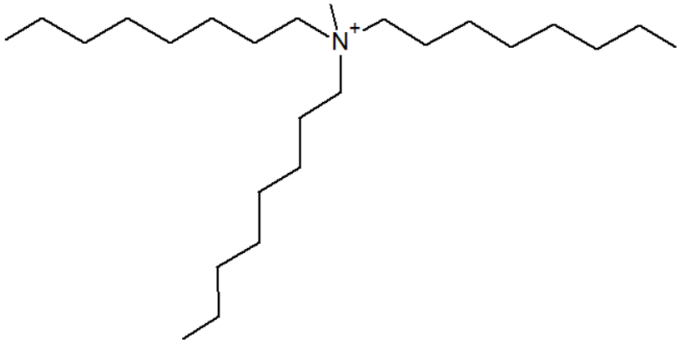
Ionic Liquids (ILs)



Imidazolium ILs

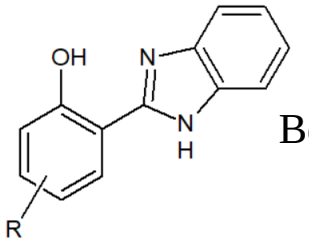


Pyridinium ILs

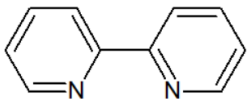


Ammonium ILs

Fluorescent Dyes

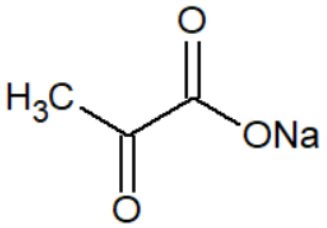


Benzimidazoles



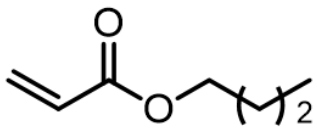
Bipyridines

Food Materials

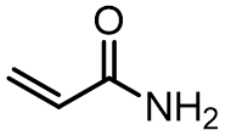


Sodium Pyruvate

Monomers



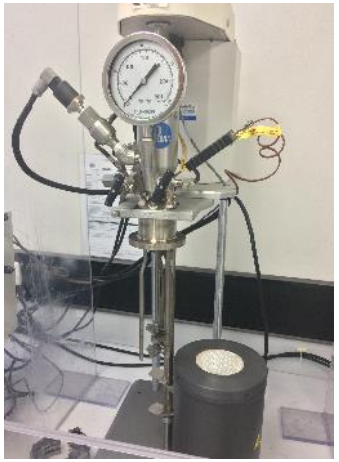
Butyl acrylate



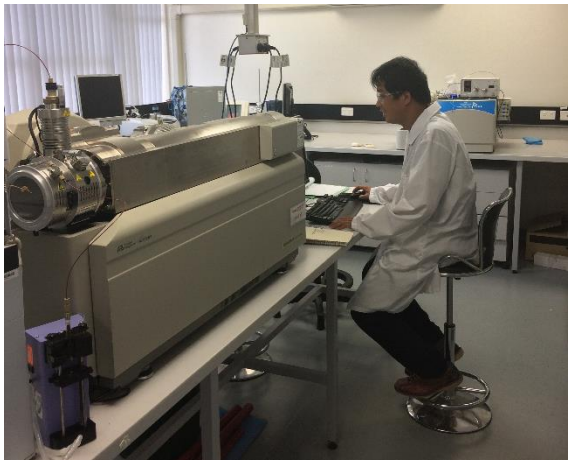
Acrylamide derivatives

Chemical Deuteration at ANSTO-NDF

Deuteration of **imidazolium** ionic liquids @ANSTO-NDF

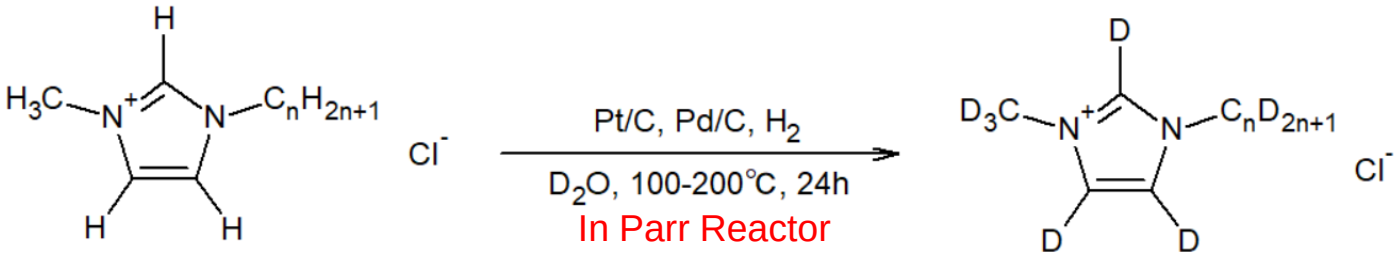


Parr Reactor



LC-MS

ANSTO-NDF staff



Deuteration Ratio

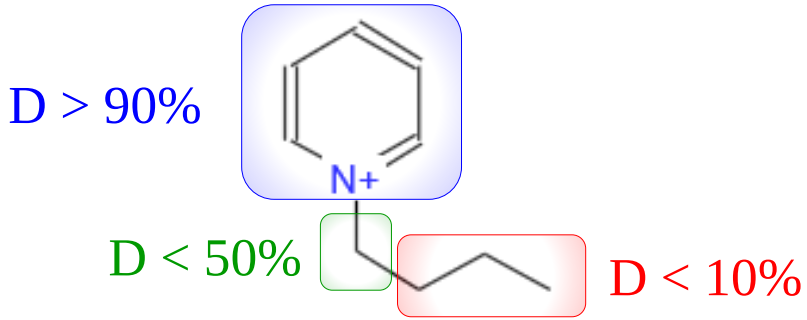
0～98%

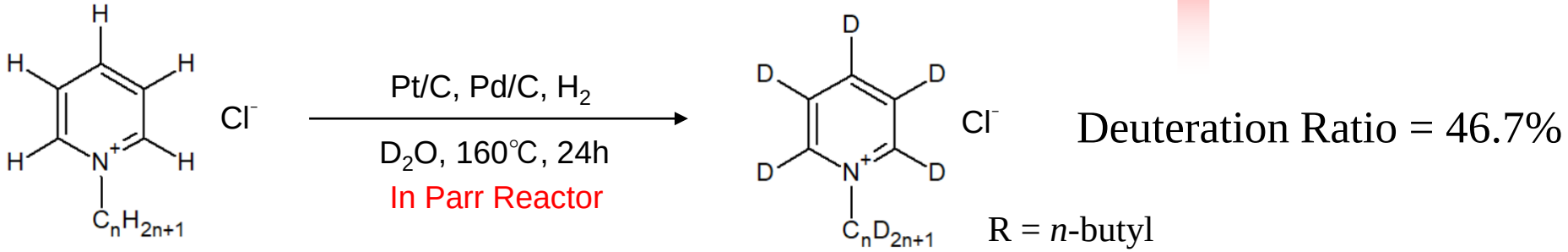
Detueration ratio controlled deuteration by one step reaction

Chemical Deuteration at CROSS_1

Deuteration of **pyridinium** ionic liquids @CROSS

Parr Reactor



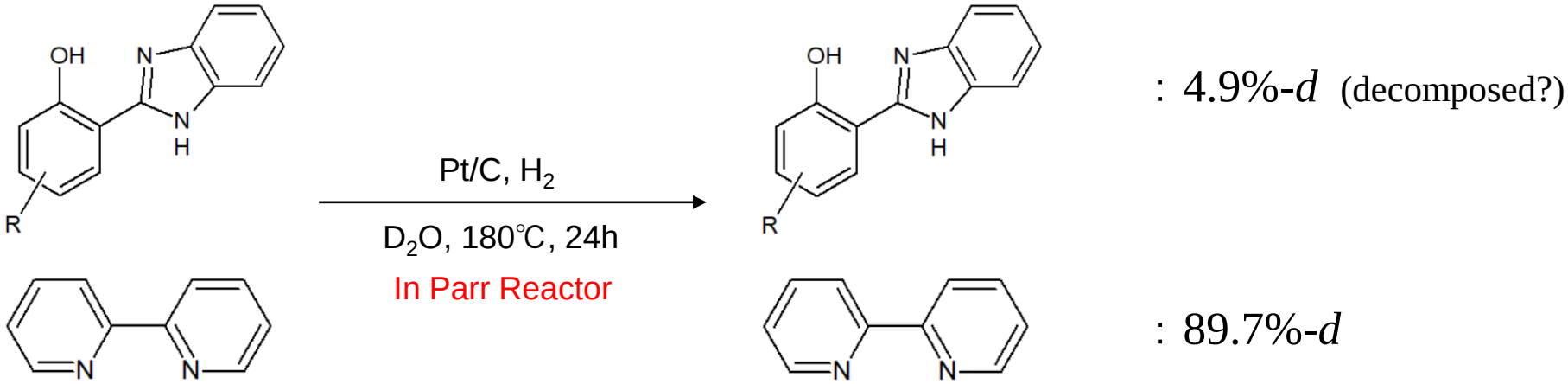


Deuteration Ratio = 46.7%

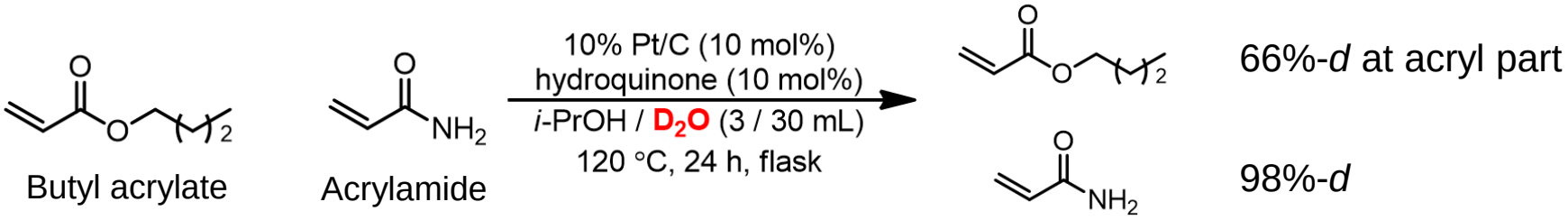
R = *n*-butyl

Chemical Deuteration at CROSS_2

Deuteration of **fluorescent dyes** @CROSS



Deuteration of **monomer** compounds @CROSS



*K. Park, *et al*, *Adv. Synth. Catal*, 2303 (2018).

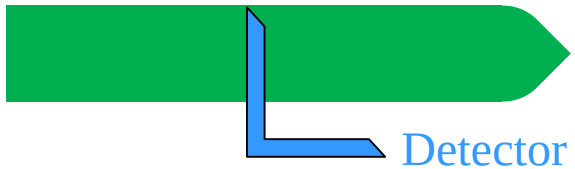
Chemical Deuteration at CROSS_3

Development of elemental analysis method

*K. Akutsu, *et al.*, *JPS. Conf. Proc.*, **25**, 011018 (2019).

$C_wD_xO_yN_z$

CO_2, H_2O, D_2O, NO_2



Detection sensitivity
$H_2O \fallingdotseq D_2O$

H/D correction formula can be expressed as*

$$\text{Corrected H\%} = AV_H \times R_H/(R_H + R_D \times 1.028) \quad (1)$$

$$\text{Corrected D\%} = AV_H \times R_D \times 1.028 \times 1.944/(R_H + R_D \times 1.028) \quad (2)$$

This is a collaboration work by CROSS and Japan Spectroscopic Corporation (JASCO)

Summary

- Deuteration of **Ionic Liquids**, **Fluorescent Dyes, and Monomers** have been carried out at CROSS.
- Various kinds of the deuterated materials are used **in inelastic (quasi-elastic) neutron scattering**, **SANS**, and **NR** experiments at J-PARC MLF

Acknowledge

I wish to acknowledge the contribution of ANSTO-NDF, Gifu Pharm. Univ., JASCO, JAEA, and CROSS to the deuterateion works.