Muon-site Calculation on $Ce(Ru_{1-x} Rh_x)_2 Al_{10}$

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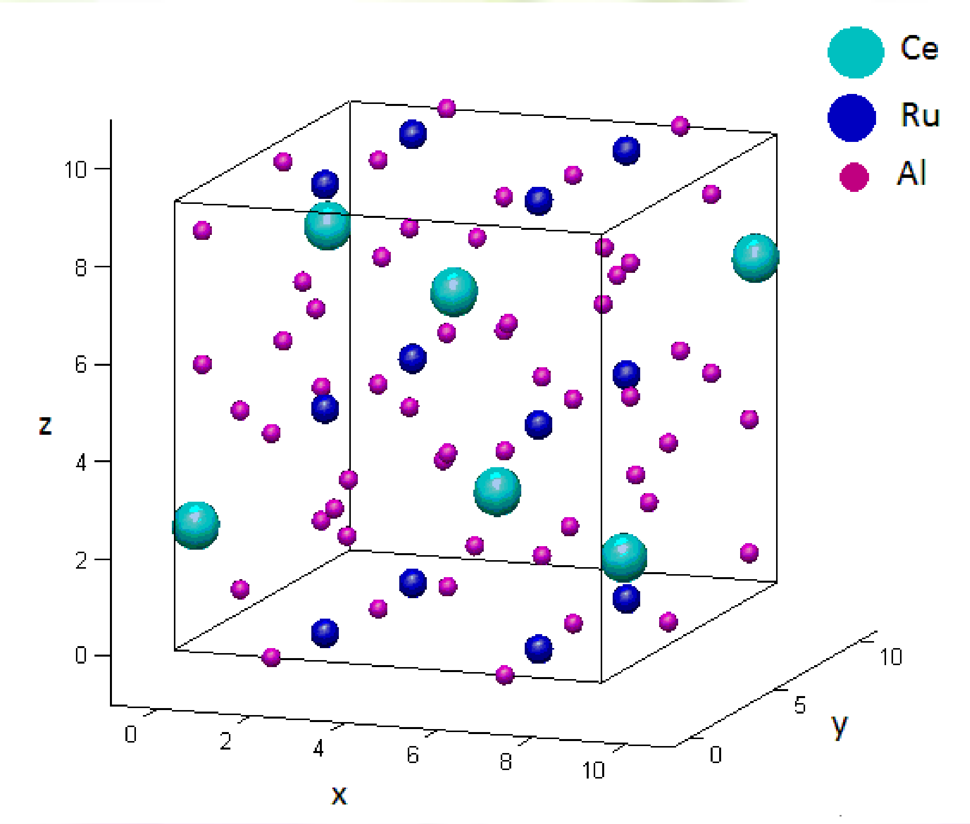
Introduction to $CeRu_2Al_{10}$

- Orthorombic structure (cmcm)
  d Ce-Ce : ~ 5.2Å



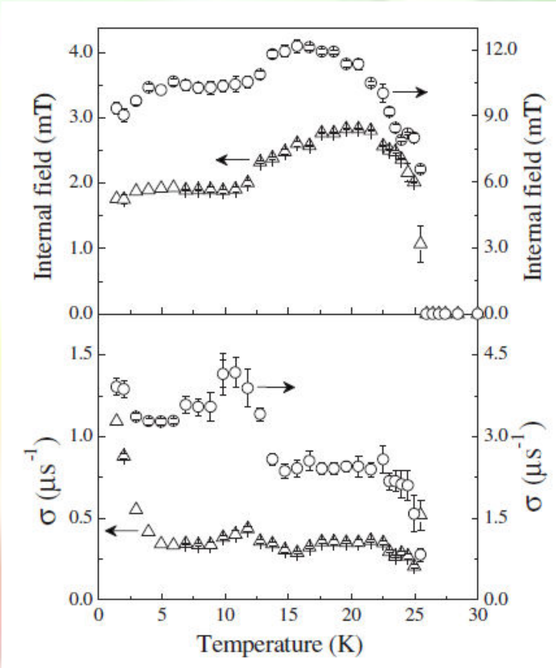
CeT_2Al_{10}	T_N	m_{AF}
T = Ru	27 K	0.42 μ_B/Ce
T = Os	29K	0.29 μ_B/Ce
T = Fe	Not ordered	

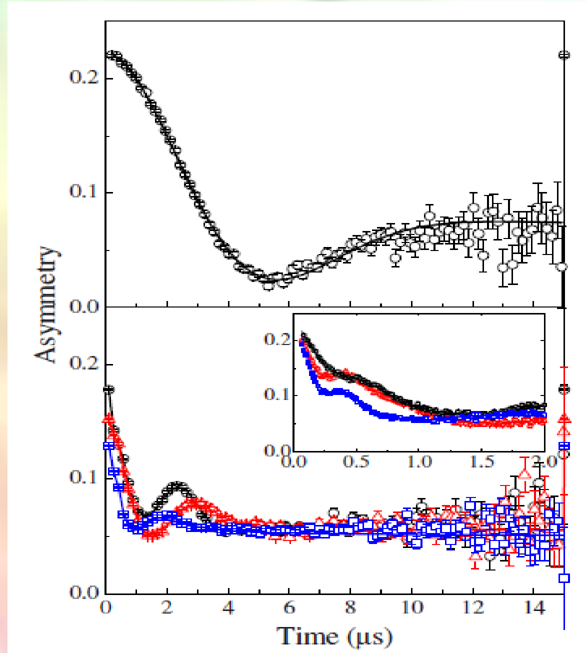
- Large anisotropy with
  $\chi_a : \chi_c : \chi_b = 13 : 4 : 1$
  m_{AF} || *c*, not *a* axis

- Spin-flop transition from m_{AF} || *c* to m_{AF} || *b* when magnetic field is beyond 4 T

- Characterized as Kondo semiconductor because of the *c*-*f* hybridization

First evidence of μSR result

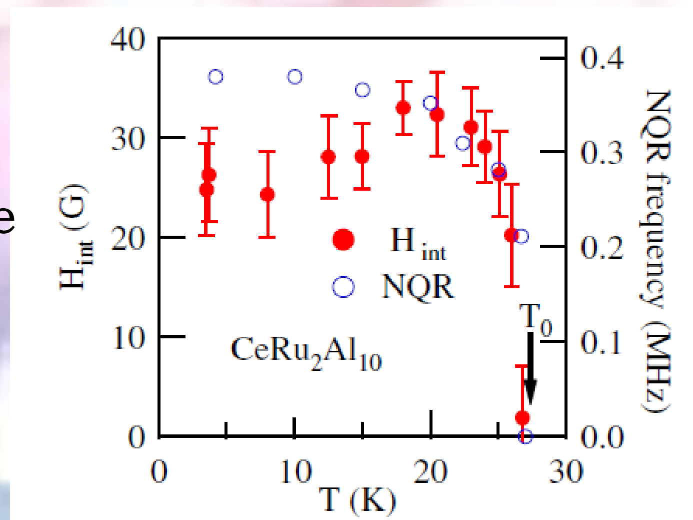


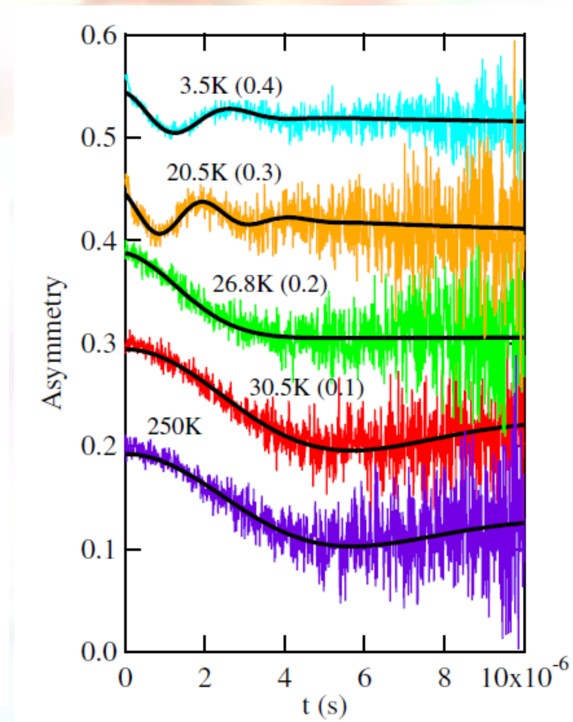


- 2 muon spin precession freq.

Khalyavin *et.al*, Phys. Rev. B 82, 100405 (2010)

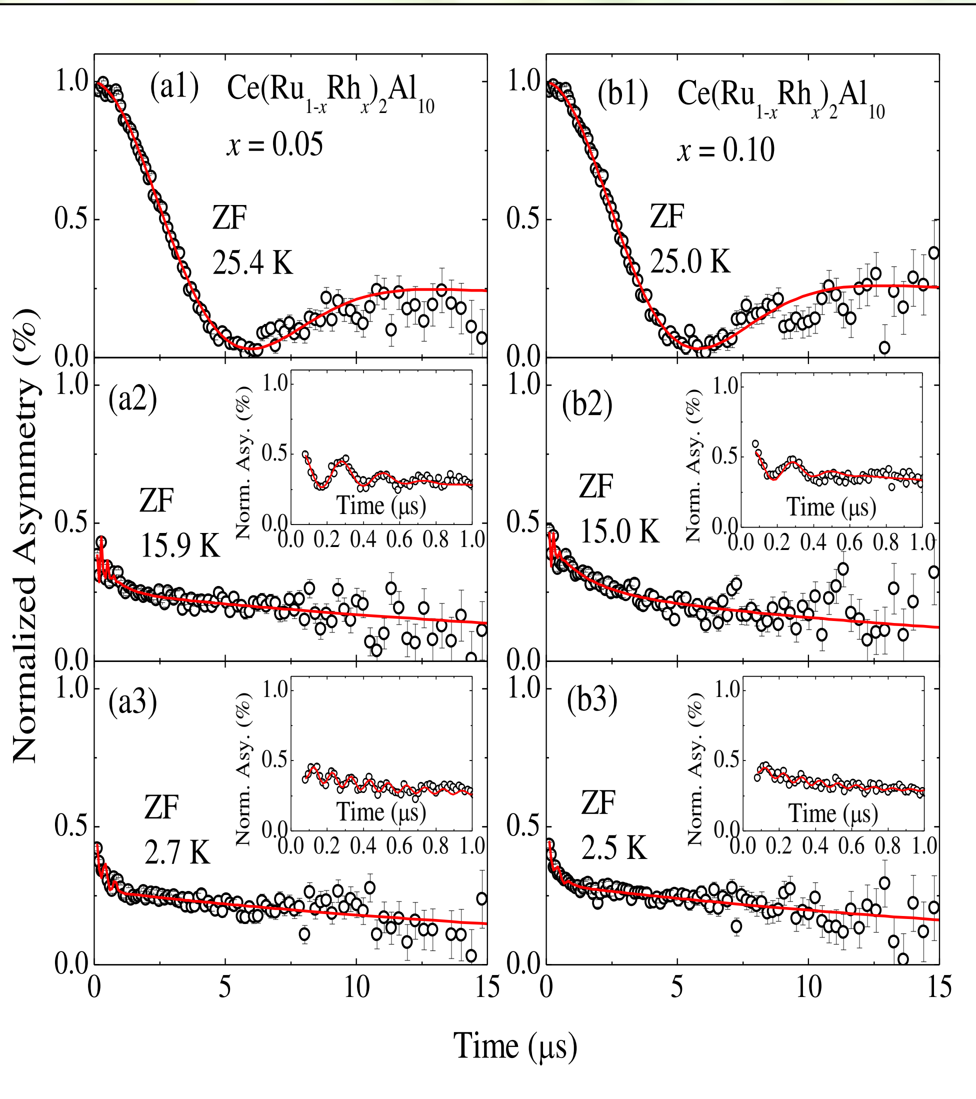
- small H_{int} at muon−site
- 4*a* site ($CeRu_2Al_{10}$)

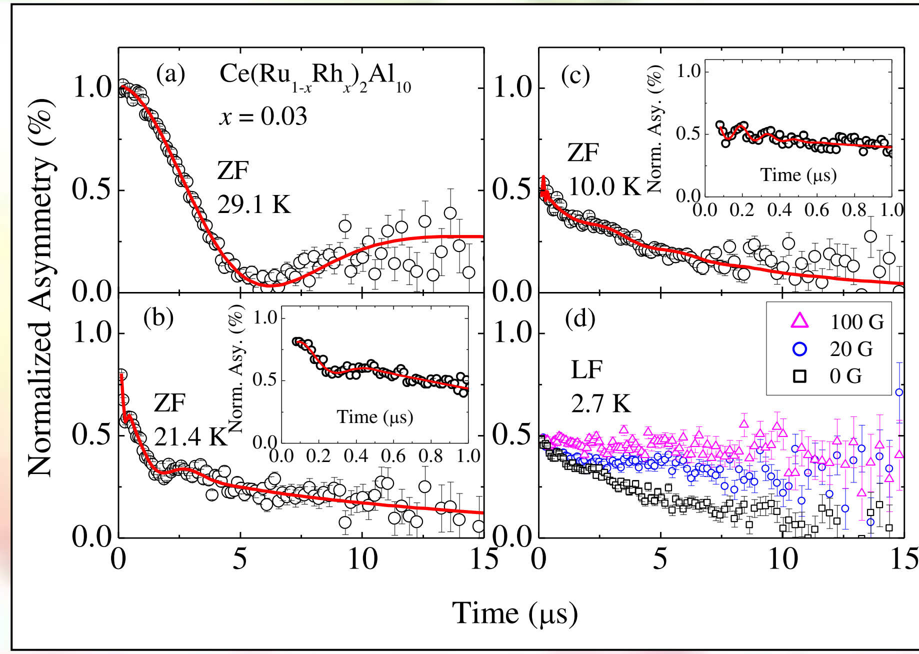




Kambe *et.al*, J. Phys. Soc. Jpn. **79**, 053708 (2010)

Introduction to $Ce(Ru_{1-x}\,Rh_x)_2\,Al_{10}$



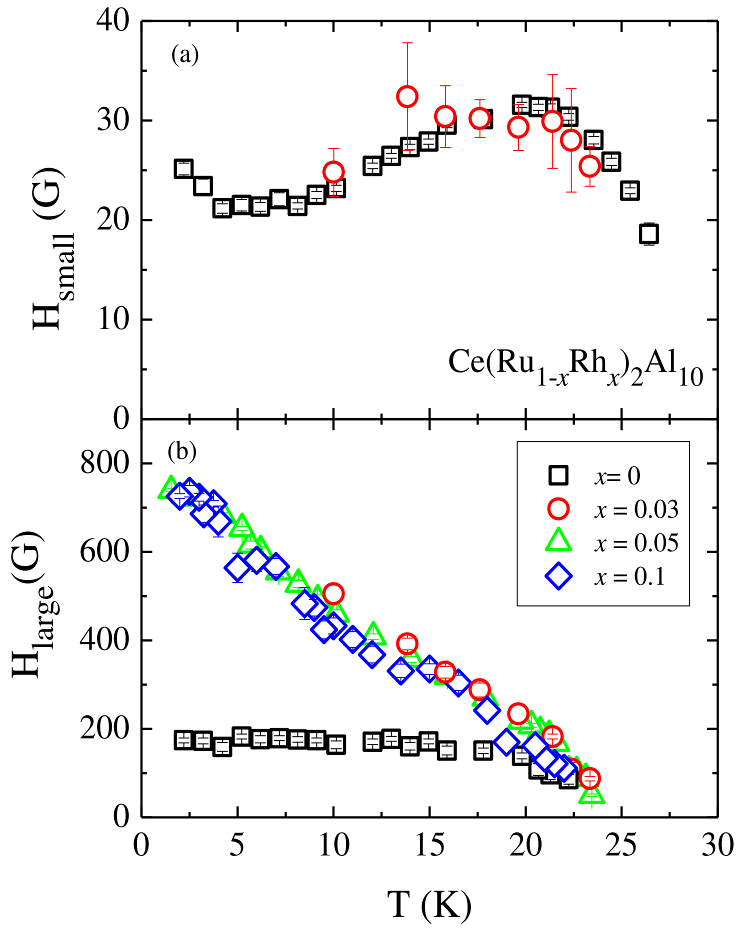


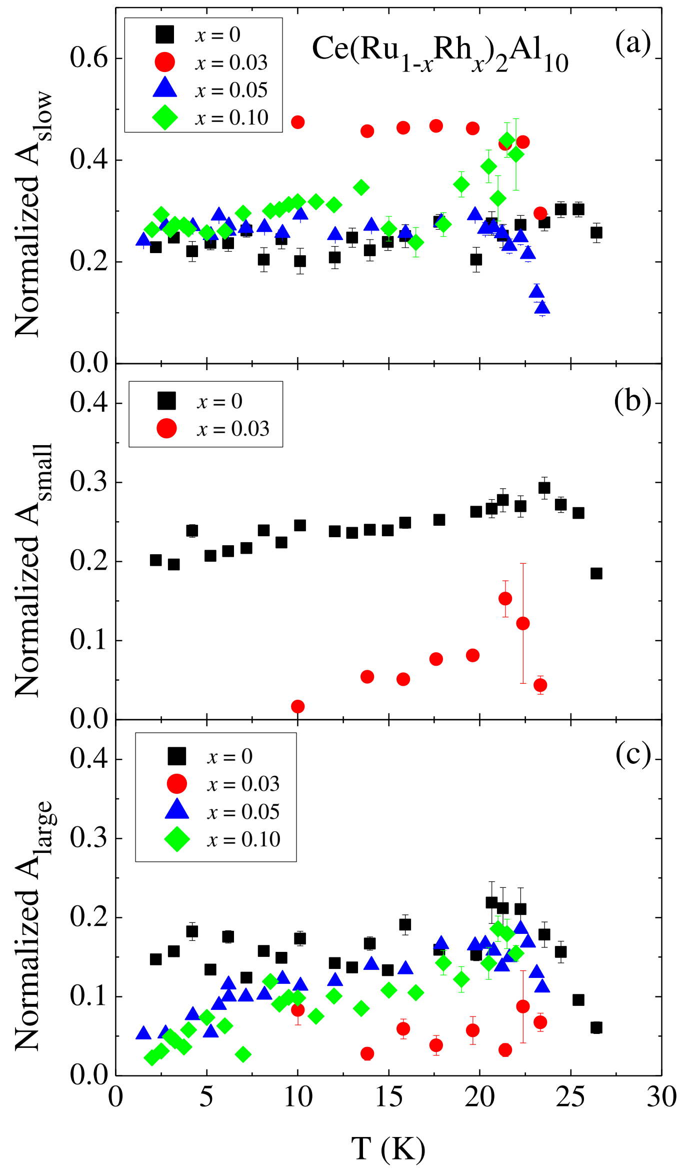
Two frequencies appear in the $x = 0$, 0.03 samples

Only one frequency in the $x = 0.05$, 0.10 samples

Guo et.al, Phys. Rev. B, 88, 115206 (2013)

Introduction to $Ce(Ru_{1-x}Rh_x)_2Al_{10}$





The internal field is changing too fast even with smallest doping of Rh

MOTIVATION

i) To understand how the magnetic moment change from a-axis → c-axis → b-axis
ii) To find out why does the internal field change so drastically even with less percentage of Rh doping.

METHOD

First attempt is :

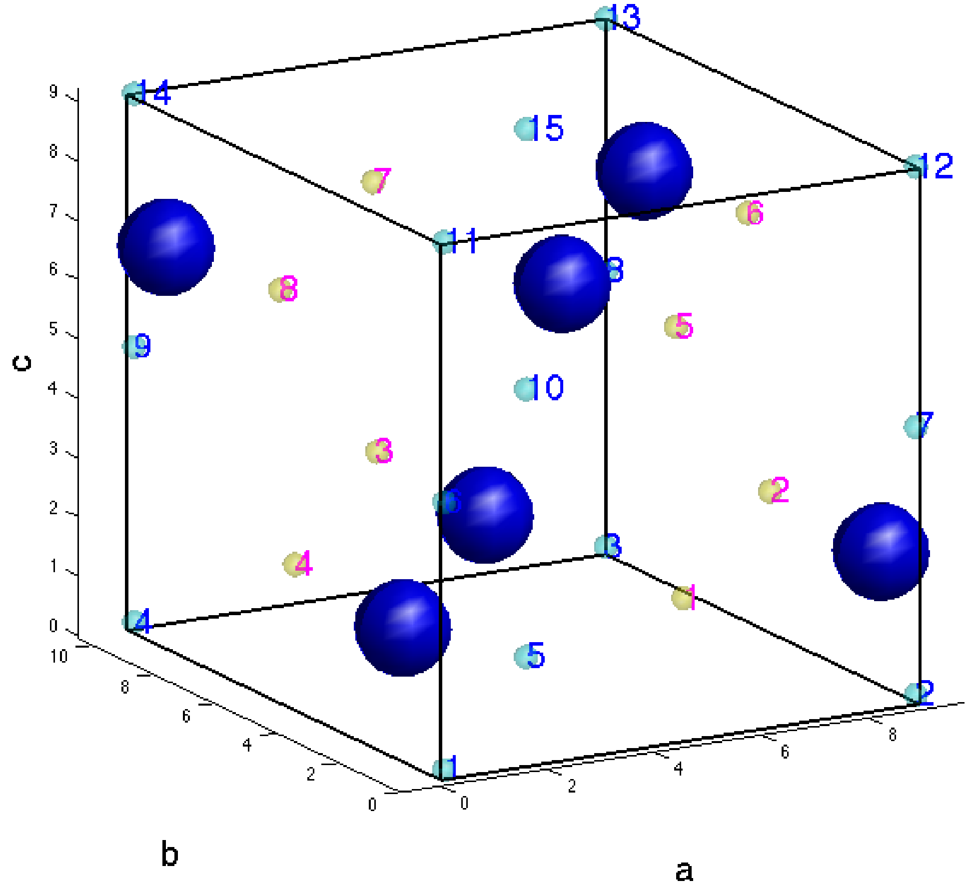
i) Find the point of minimum potential energy in the material
ii) Calculate the internal field and compare with the experimental result

Software :

i) VASP 4.5
ii) RICC
iii) MATLAB

Dipole Field Calculation

M1	Fields (G)
1	13.01
2	13.42
3	13.40
4	13.32
5	13.68
6	12.69
7	13.35
8	13.61



M2	Fields (G)
1	13.36
2	12.27
3	13.58
4	13.22
5	12.52
6	13.21
7	12.75
8	13.82
9	13.11
10	13.97
11	13.04
12	13.36
13	12.72
14	13.32
15	12.54