Nuclear Techniques for Studying Soft Matter at ISOLDE

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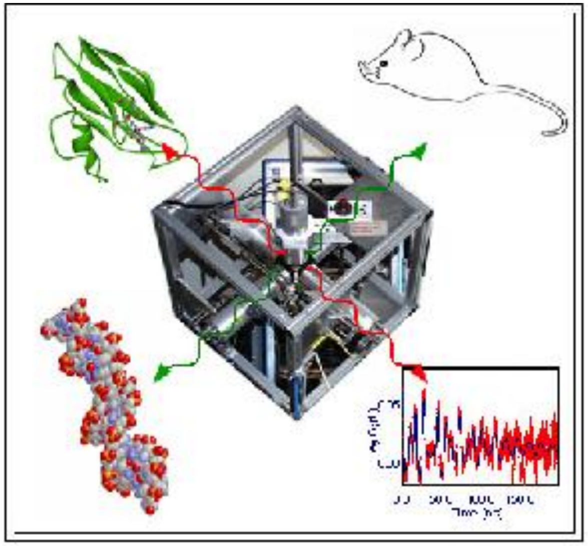
Outline

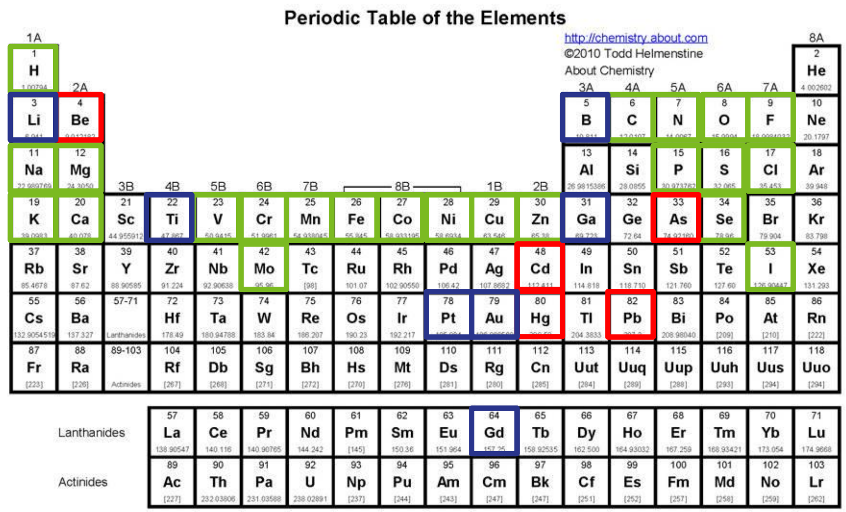
1) Motivation
2) Techniques and Experiments
3) Results
4) Outlook



Motivation

Human body:
99%: H, O, C, N
1%: 19 other elements

Motivation



- Natural elements
- Toxic elements
- Elements used in drugs

Human body:

99%: H, O, C, N

1%: 19 other elements

Techniques and Experiments

Goals:

1) Understand heavy metal ions toxicity ($Hg^{2+}$and Pb^{2+})
2) Monitor Zn^{2+} and Cu^{+} containing proteins

Nuclear and Hyperfine Interaction Techniques used in Biology:

1) Mössbauer Spectroscopy
2) ESR / EPR Spectroscopy
3) NMR Spectroscopy
4) NQR Spectroscopy
5) PAC Spectroscopy

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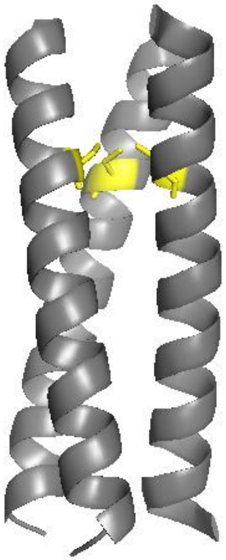
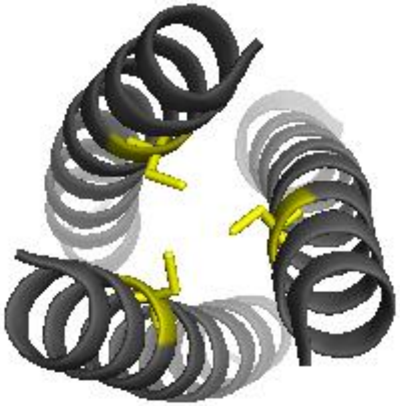
Zn(II) → Cd(II)
Cu(I) → Ag(I)

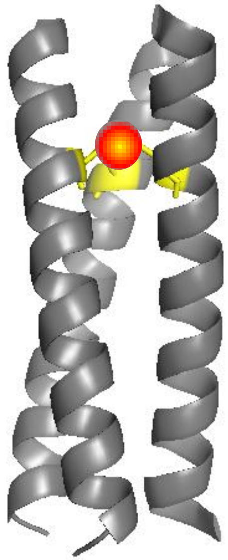
6) βNMR Spectroscopy (?)

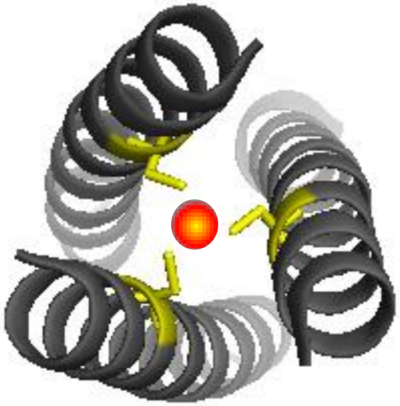
PAC Spectroscopy



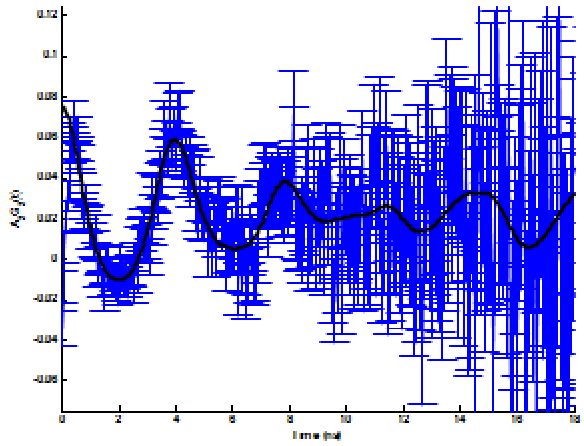


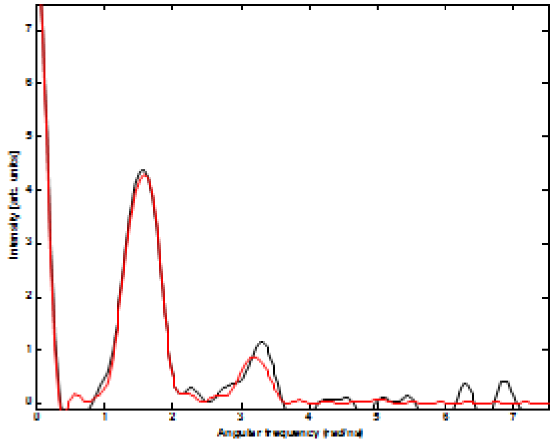
PAC Spectroscopy





199mHg-PAC Spectroscopy on *de novo* synthesized peptides





PAC Spectroscopy

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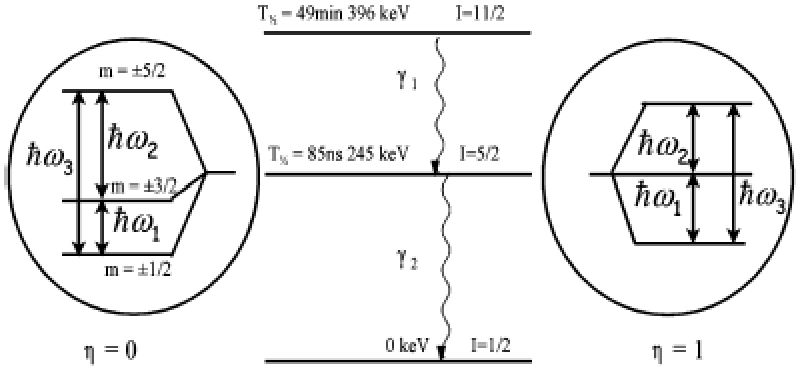
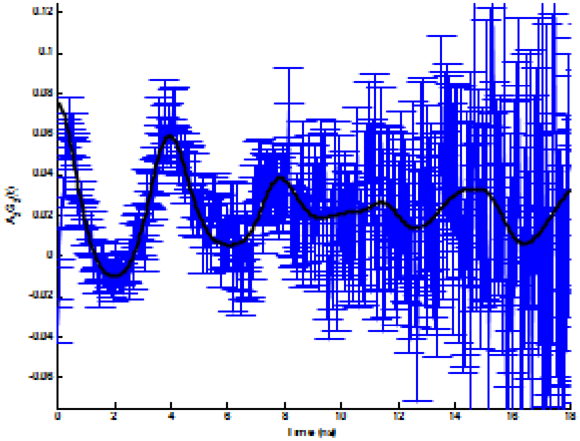
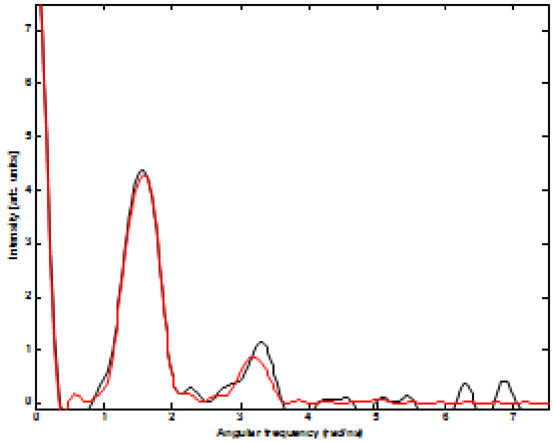
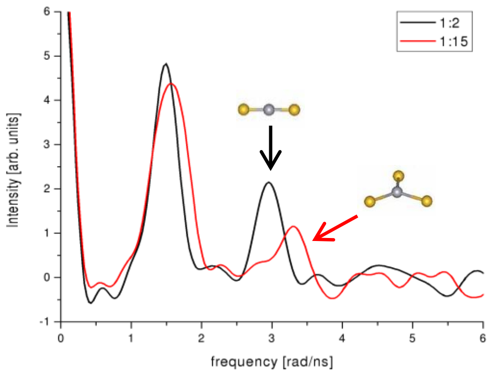


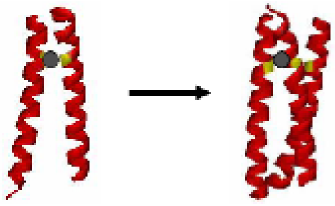




PAC Spectroscopy

Metal : peptide ratio
1:2 → 1:15





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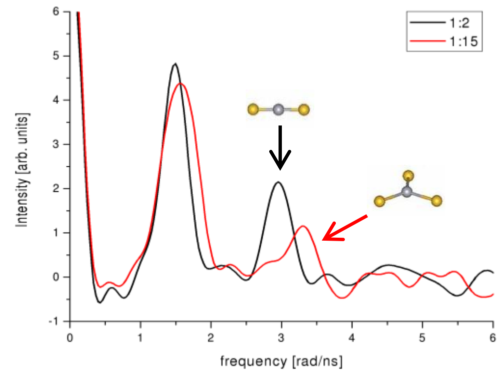
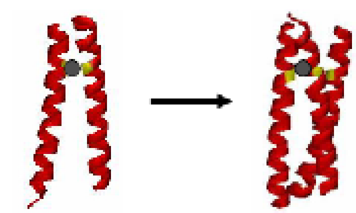
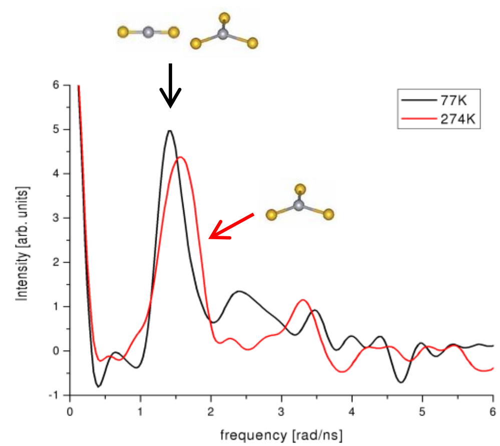
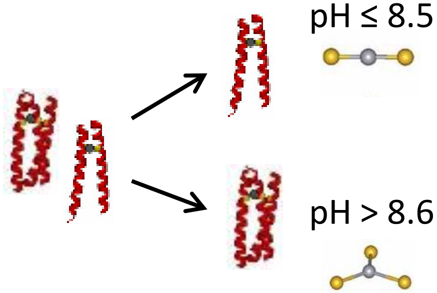




Temperature and pH
77K → 274K
8.5 → 9.4





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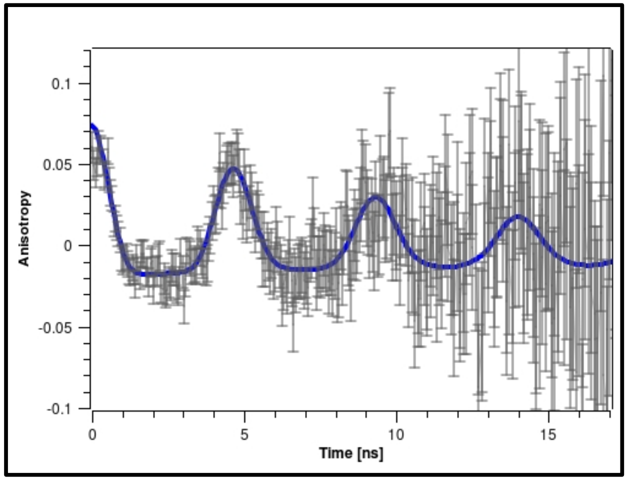

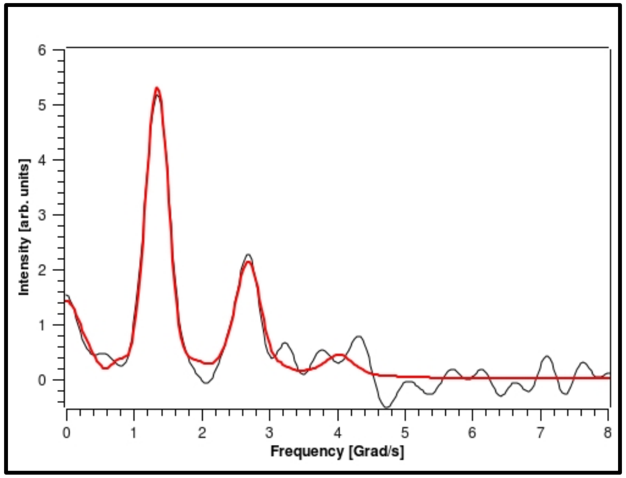

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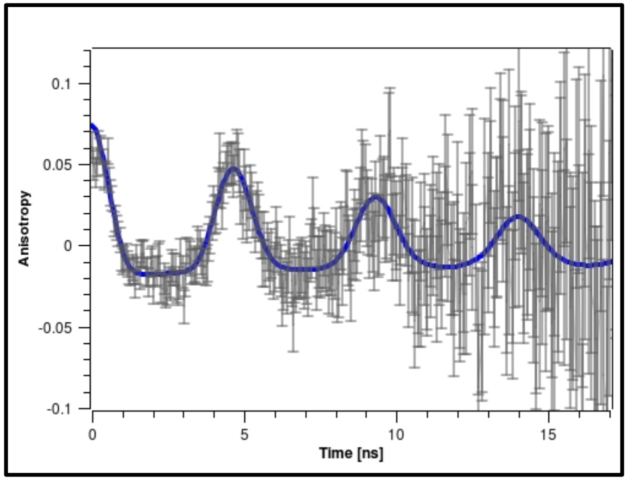
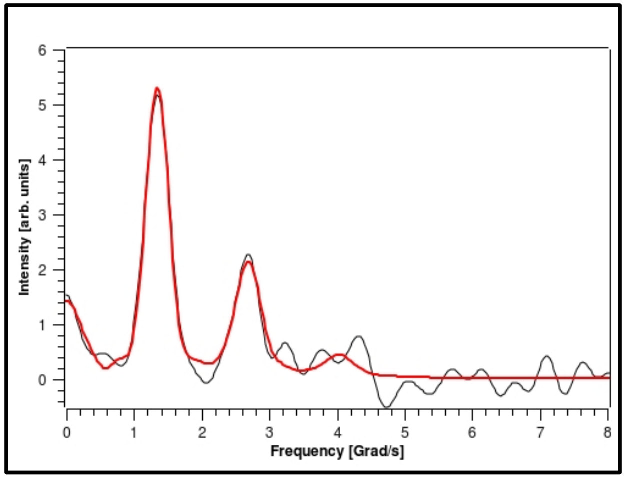




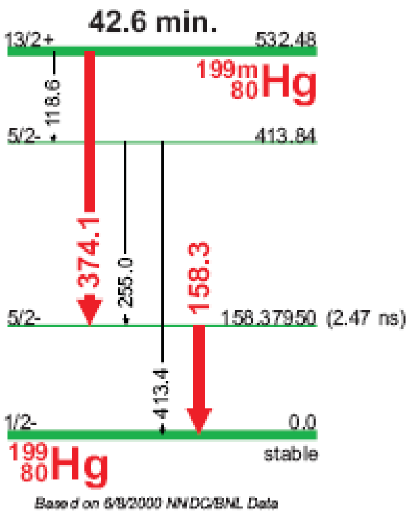
PAC Spectroscopy

Advantages:

- Characterisation of structure and dynamics at the PAC probe site
- High sensitivity to structural changes
- Small amount of PAC probe needed (in principle about 1 pmol)
- Different physical states: crystals, surfaces, solutions, *in vivo*...

Limitations:

- Suitable PAC isotopes do not exist for all elements
- PAC isotope must bind strongly to the molecule
- After effects can cause problems
- Production of PAC-isotopes



Hemmingsen et al. *Chem. Rev.*, **2004**, 104: 4027

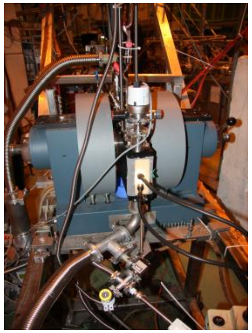
Hemmingsen and Butz, in "Application of Physical,Methods to Inorganic and Bioinorganic Chemistry" **2007**

βNMR Spectroscopy

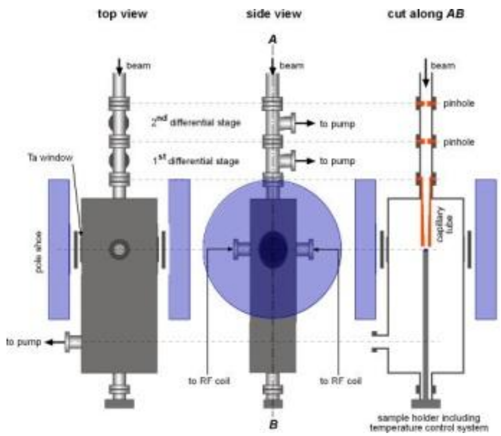
- Measurement: beta decay anisotropy
  - chemical shifts
  - quadrupole interactions (also time dependent)
- Advantage: physics and data analysis basically the same as for “standard” NMR
- Disadvantage: localization

βNMR vs “standard” NMR

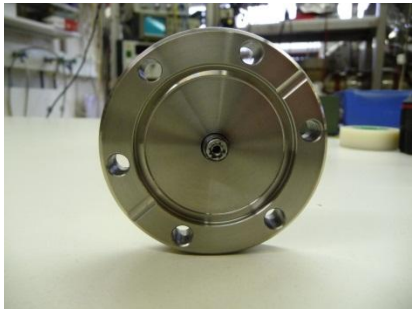
Property	NMR	βNMR
polarization	mag. field	polarized beam
isotopes	stable	radioactive
number of nuclei	10^{18}	10^{8}
nuclear polarization	small	10 – 100%
magnetic field	yes	yes / no
type of experiment	offline	online



βNMR Spectroscopy: Setup



Pinholes



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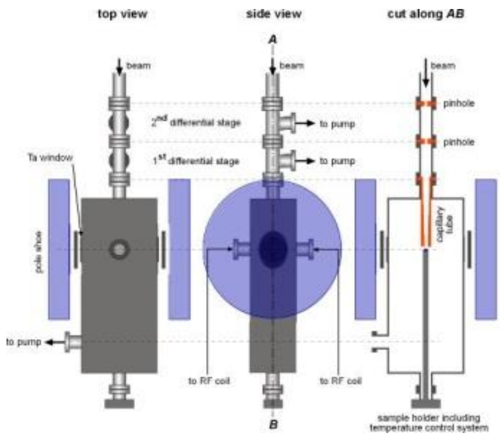

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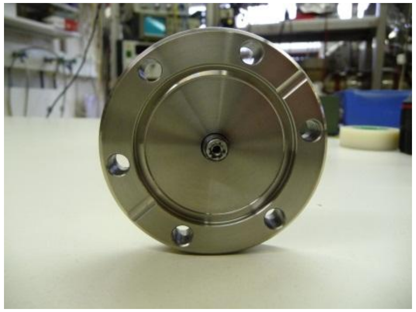
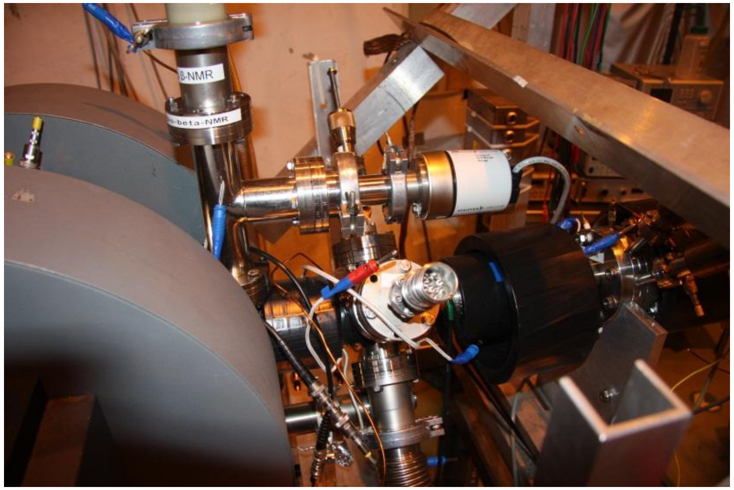


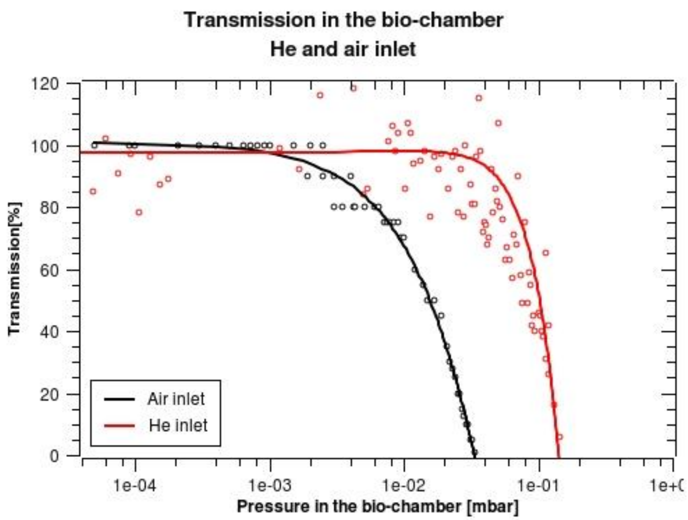
Chamber

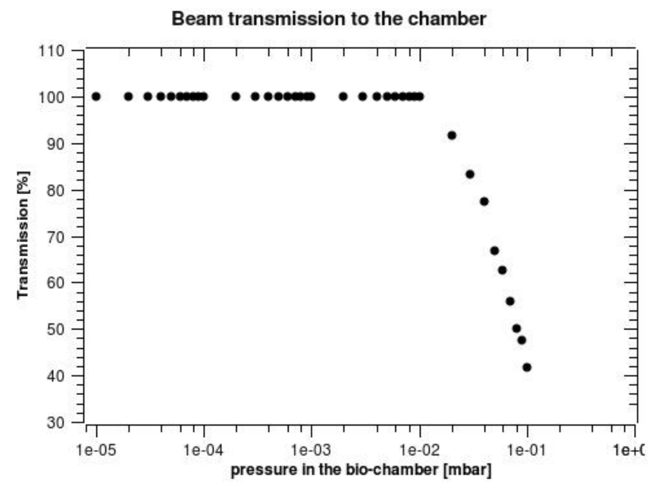
At the COLLAPS magnet



βNMR Spectroscopy

Beam Transmission to the chamber:





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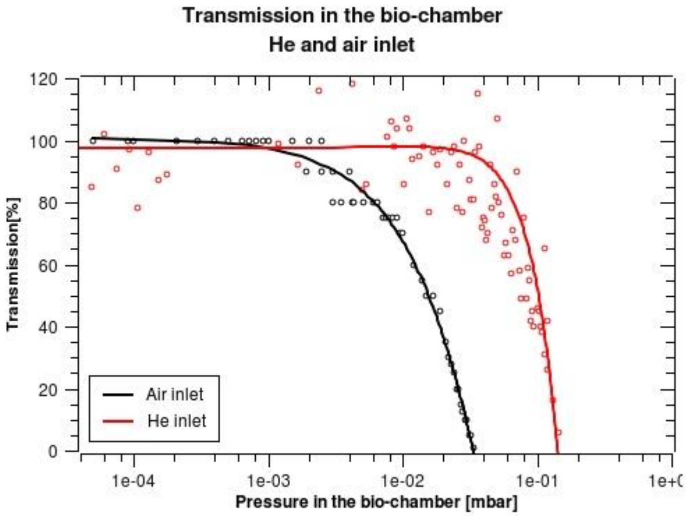

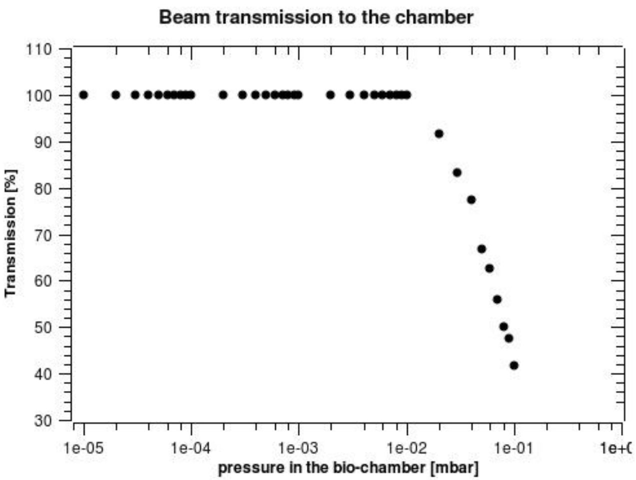

- Guiding through pinholes (~10%)
- Magnetic field at nominal value (100%)
- Guiding field on (100%)
- He inlet, 2·10-2 mbar (100%)
- Liquid droplet maintained in the chamber (100%)

Setup ready for radioactive beam

Outlook

PAC Spectroscopy:

- Studies of heavy metal ion binding to proteins and nucleic acids (RNA/DNA)
- Water purification by bacteria
- Heavy metal ion binding by plants and bacteria (in vivo experiments)
- Record the first clearcut ^{204m}Pb PAC for proteins

βNMR Spectroscopy:

- First experiments on ^{31}Mg in Aug 2012
  - different liquid
  - small molecules
  - proteins or RNA
- Setup optimization

Fundings

CERN

Bundesministerium für Bildung und Forschung

Danish Agency for Science Technology and Innovation
Ministry of Science Technology and Innovation

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République Française
Ambassade de France au Danemark

DCSC Danish Center for Scientific Computing

VILLUM KANN RASMUSSEN FONDEN & VELUX FONDEN

Thank you!