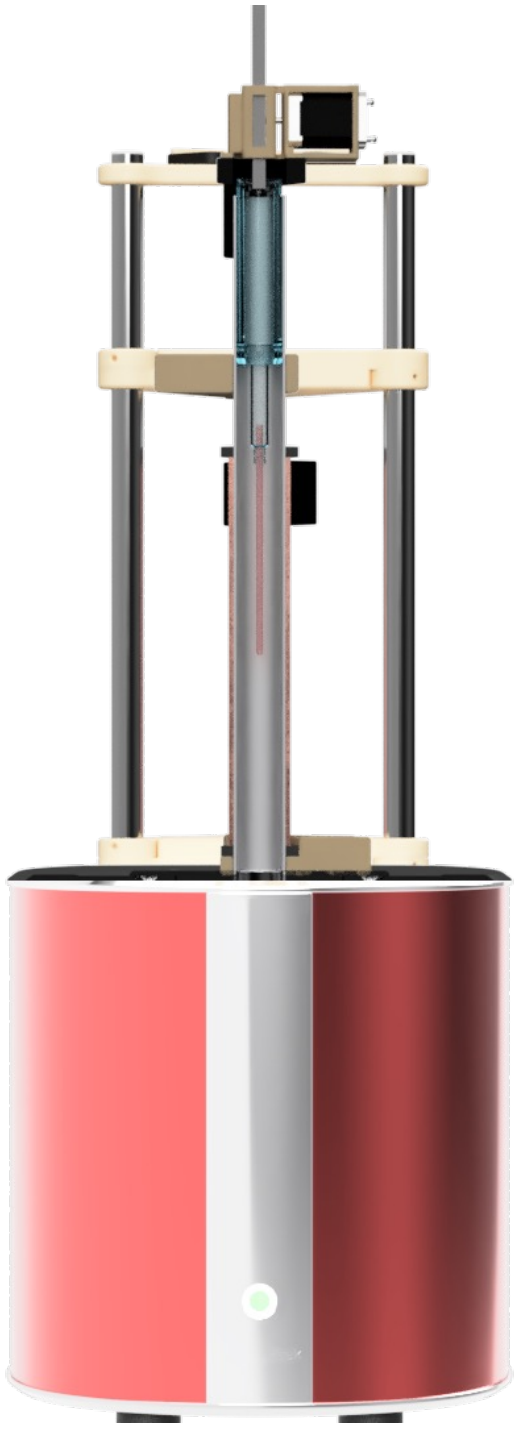
Low-cost magnetic field cycling system for benchtop NMR spectrometer



Christian-Albrechts-Universität zu Kiel

GRK 2154 Materials for Brain

MOIN CC molecular imaging north competence center

UKSH

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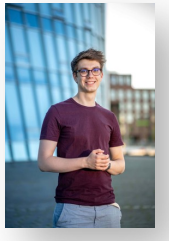


Frowin Ellermann

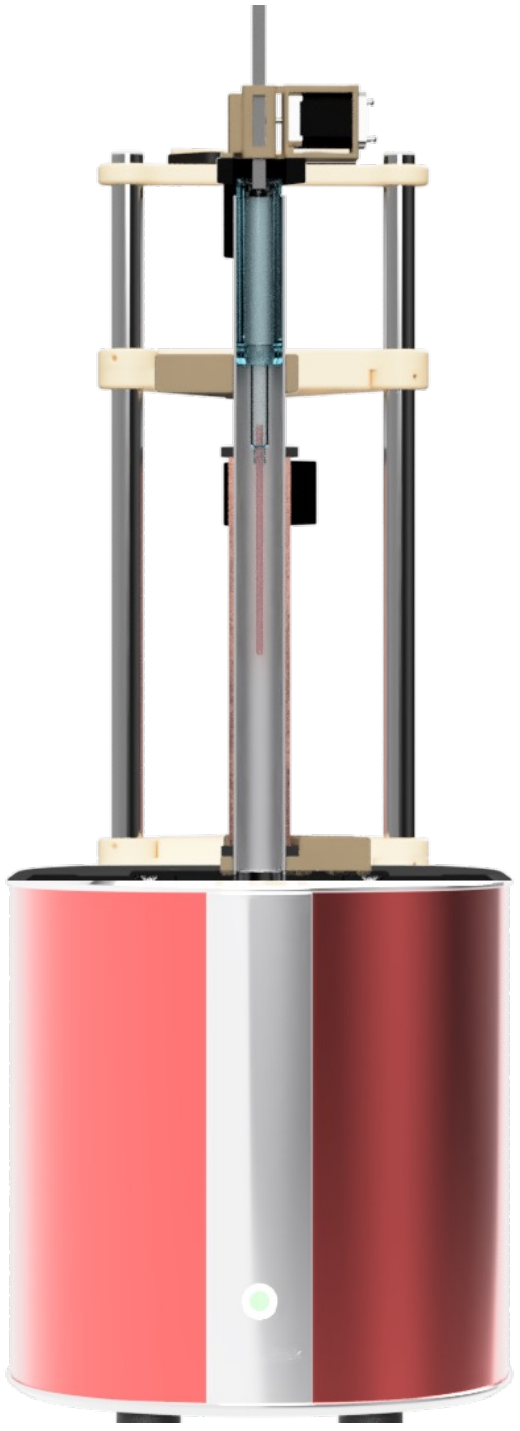
PhD student in engineering

at MOIN CC (University Hospital Kiel, Germany)

Wednesday,
October 13th 2021

or as we call it …

field alternation setup for a compact NMR spectrometer (FALCON)



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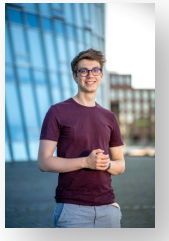

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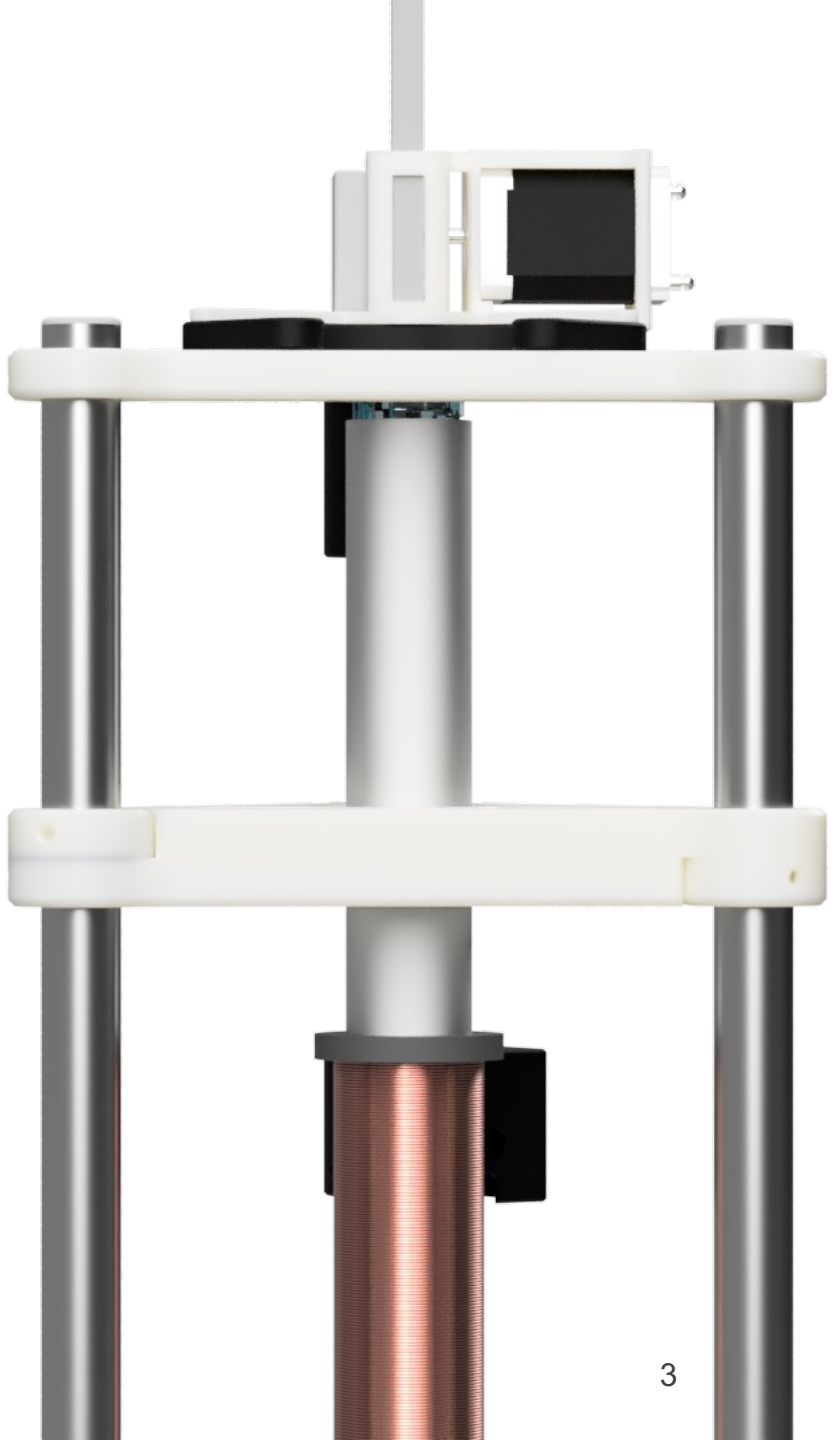
Agenda

deconstruction of the title

about hardware

about software

about applications



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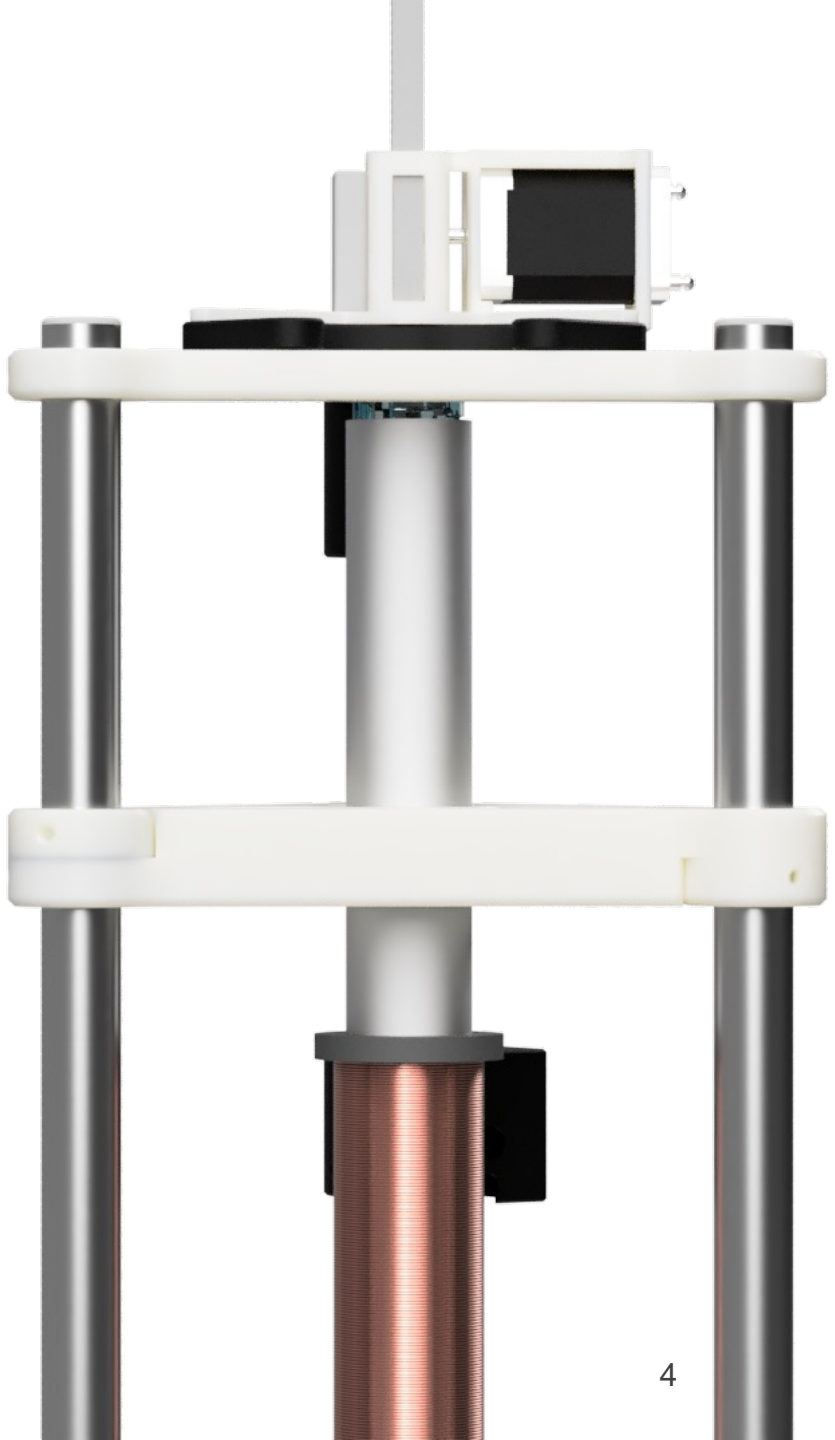
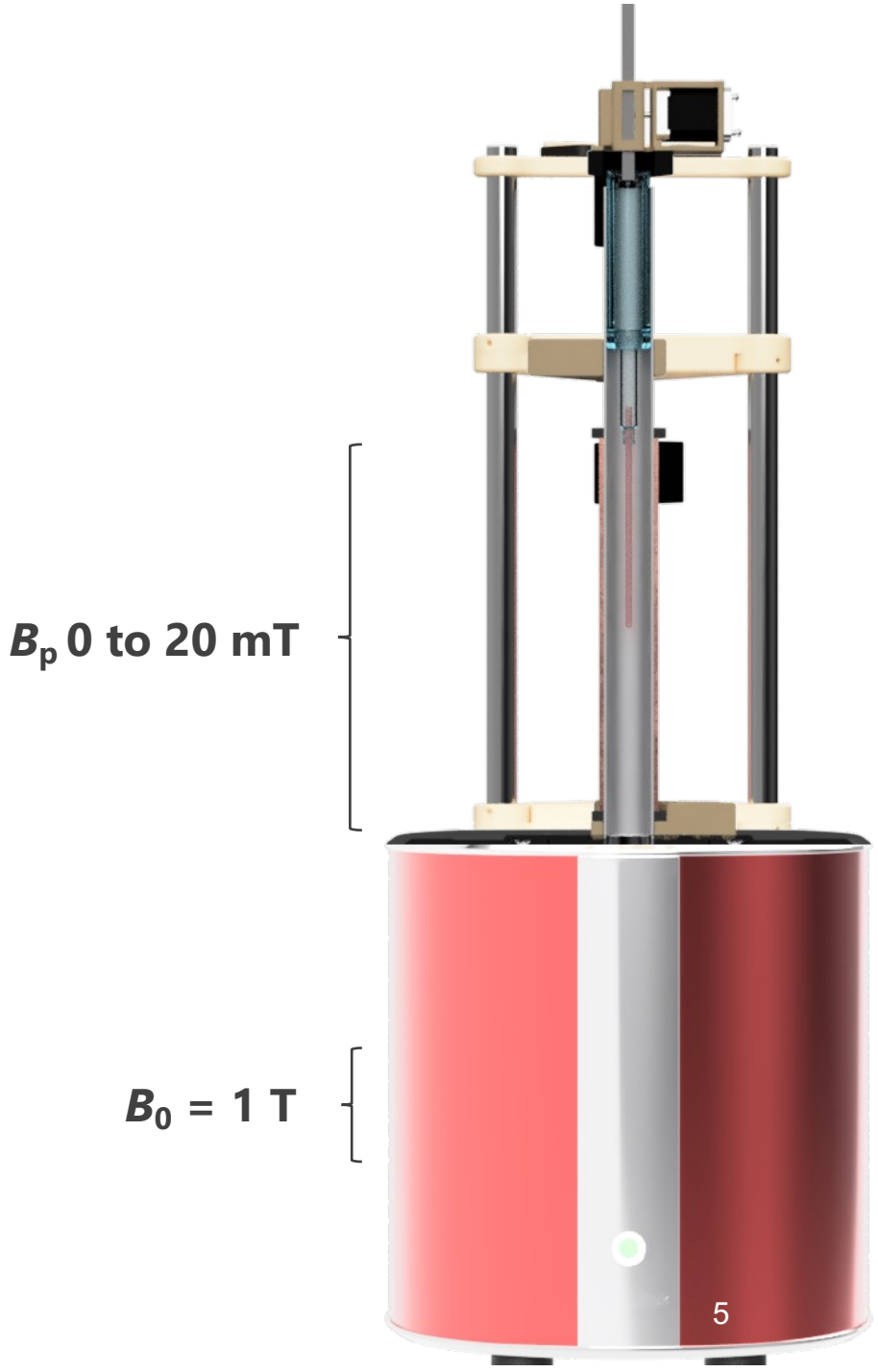


Low-cost magnetic field cycling system for benchtop NMR spectrometer

here, in case of parahydrogen-induced hypolarization (PHIP), magnetic field cycling refers to polarization in field B_p and signal acquisition in field B_0.



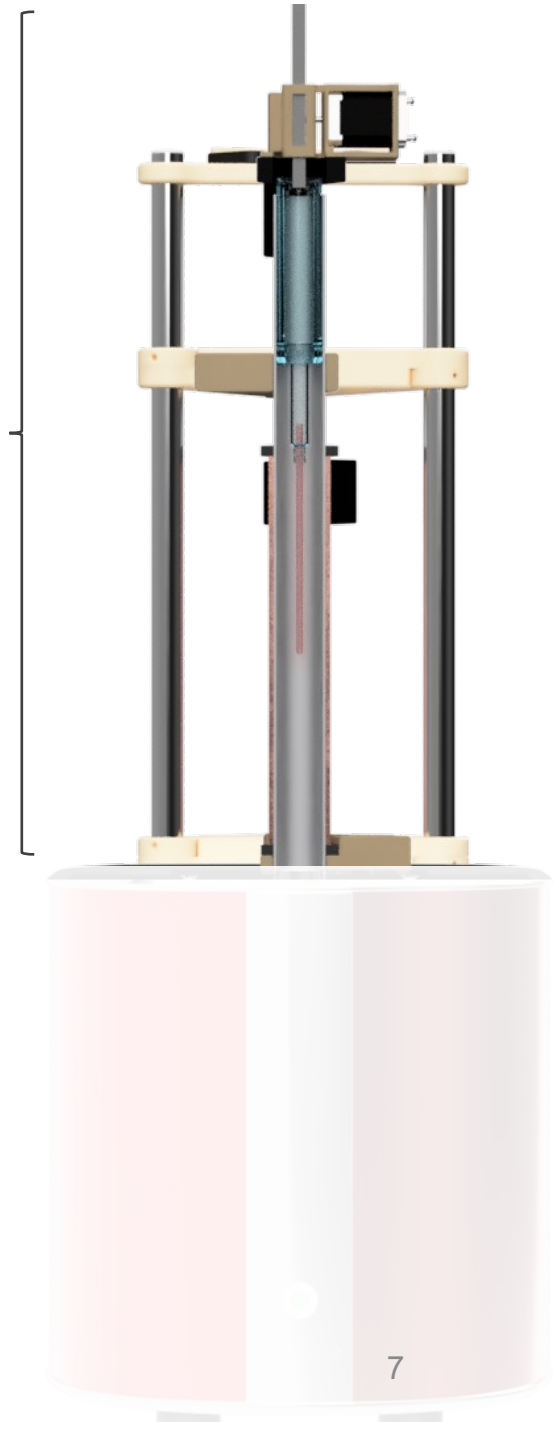
Low-cost magnetic field cycling system for benchtop NMR spectrometer

Why benchtop NMR spectrometer?

- they are affordable
- they are compact and ideal for putting setups on top
- main drawback (low field) is neglectable for hyperpolarization experiments

Low-cost magnetic field cycling system for benchtop NMR spectrometer

Cheap! Cheap!
< $500



Low-cost setups are great for groups who want to enter the field of hyperpolarization. But what makes them so affordable?

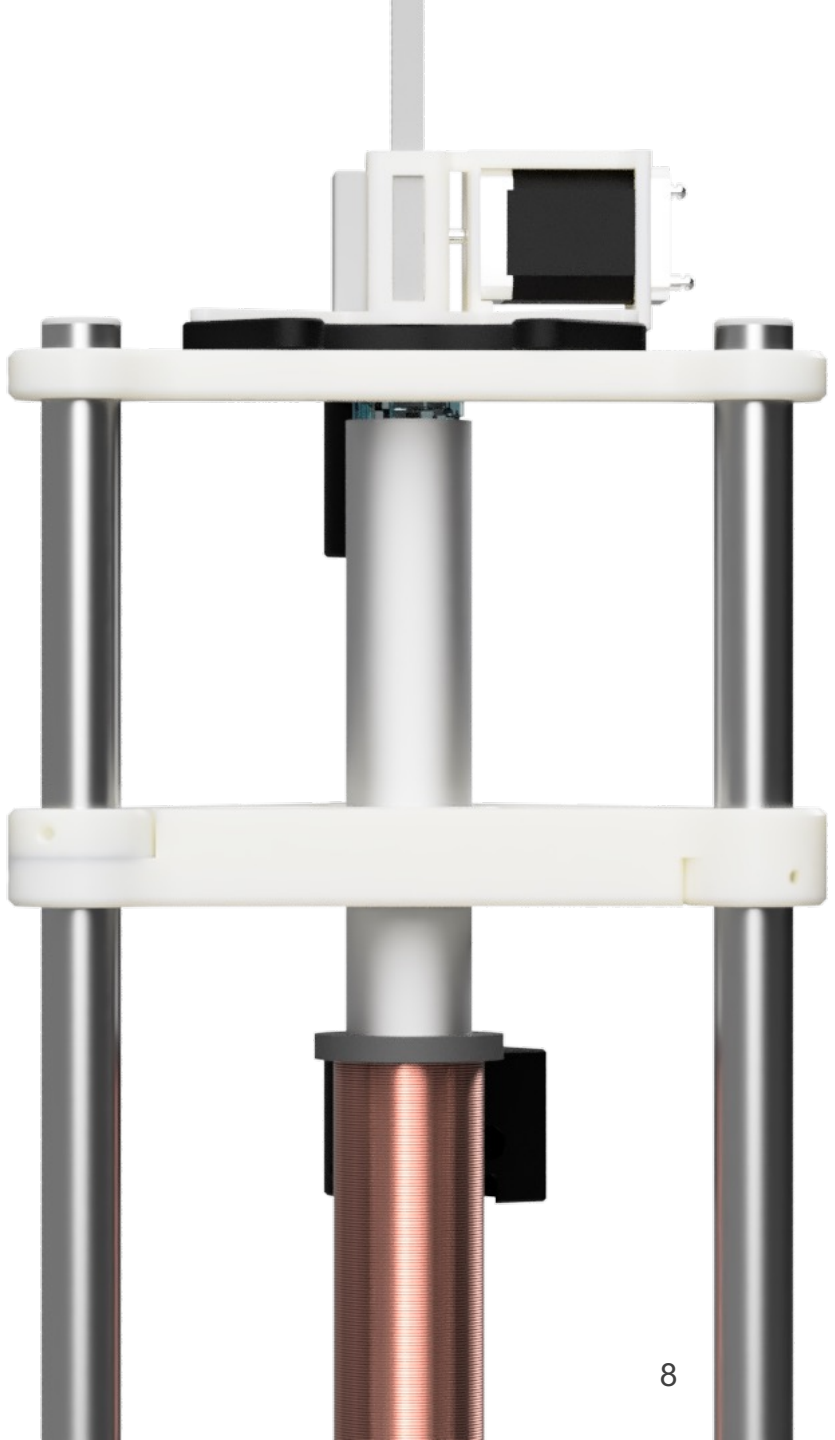
- benchtop NMRs are - comparably – affordable $$$
- rapid prototyping technologies as 3D-printing makes it accessible and cheap
- no specialized workshop needed & use of off-the-shelf parts

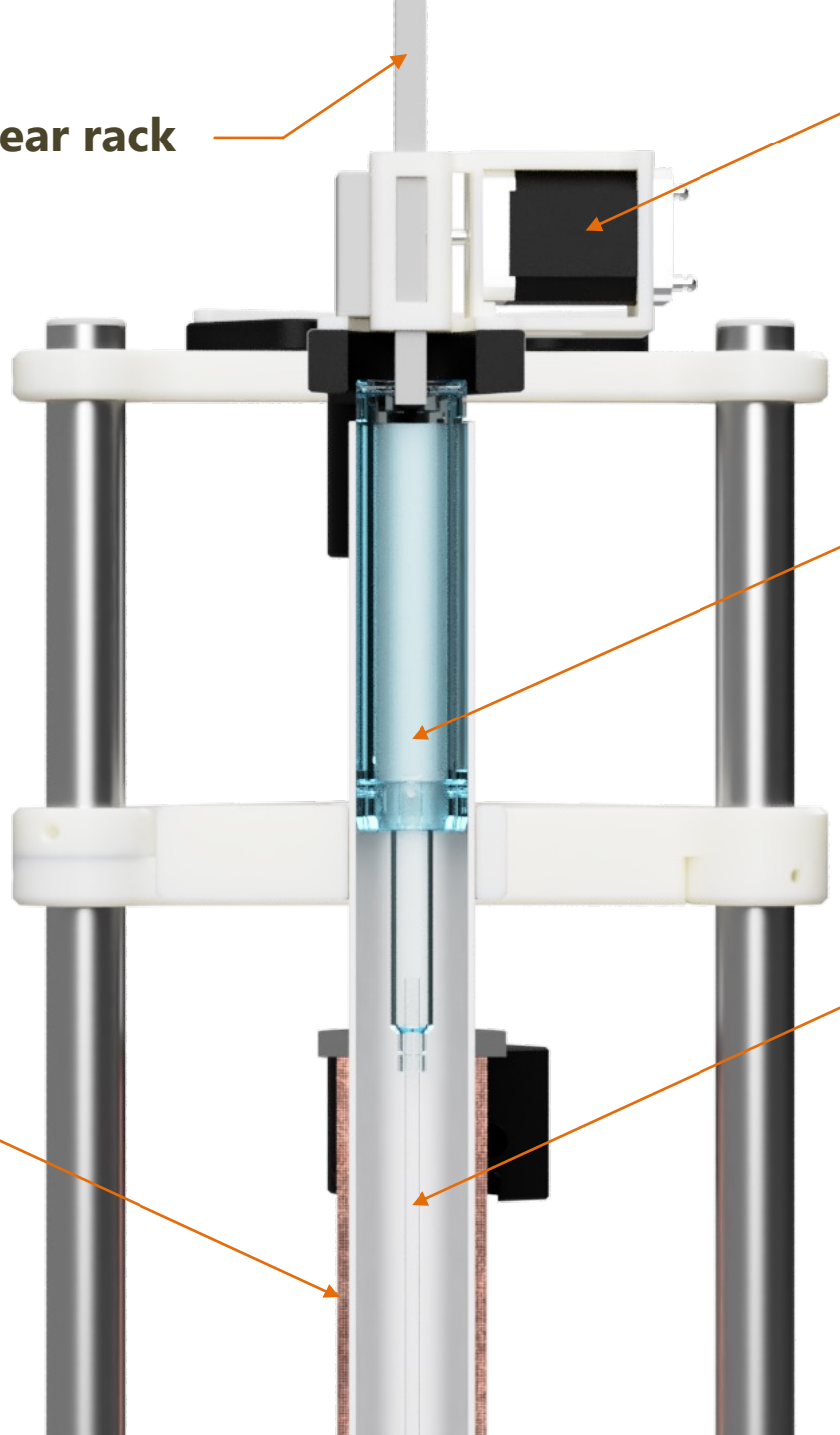
deconstruction of the title

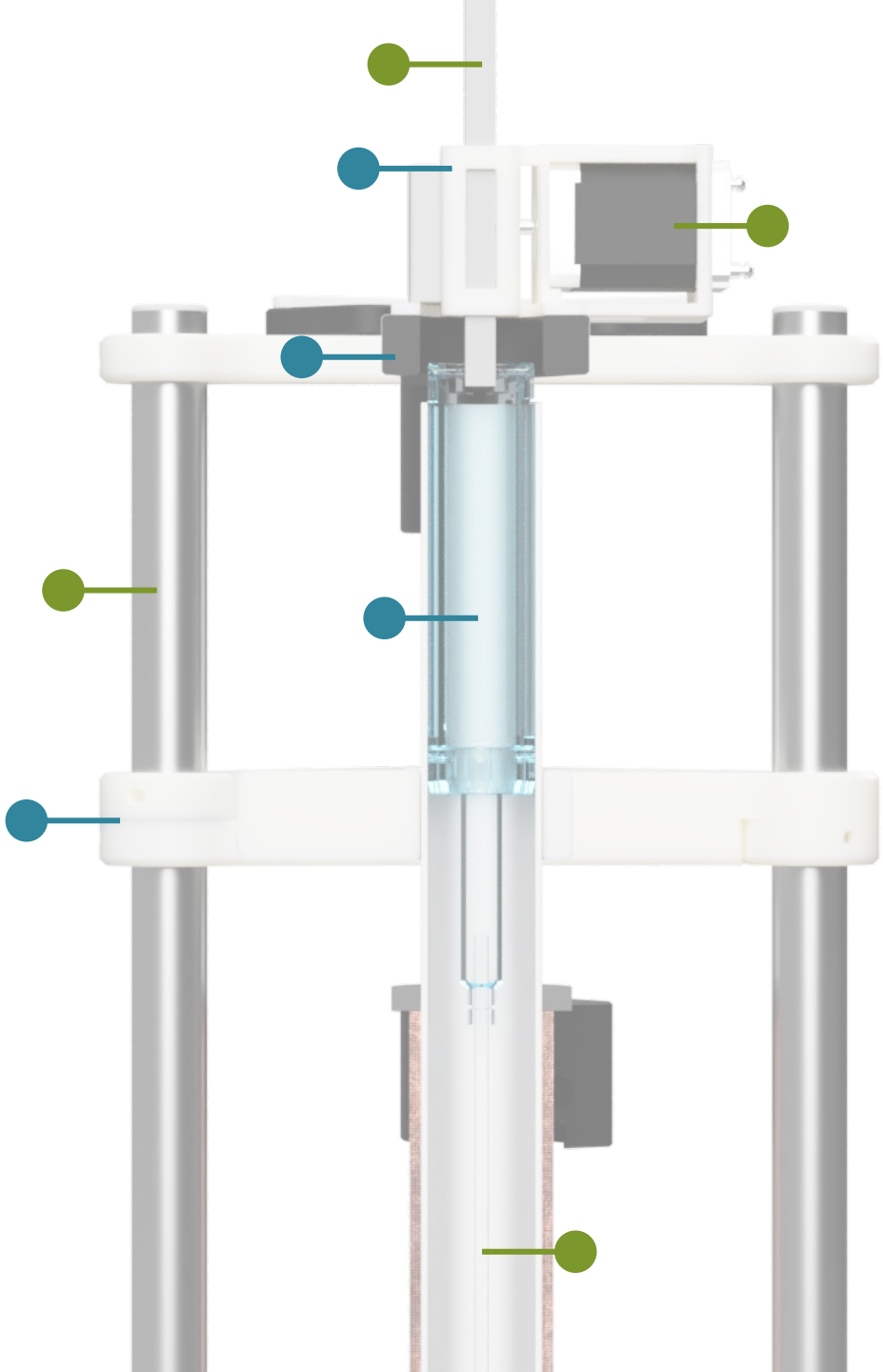
about hardware

about software

about applications




gear rack
stepper motor
NMR tube carrier
5mm NMR tube
resistive polarization coil
B_p = 0 – 20 mT

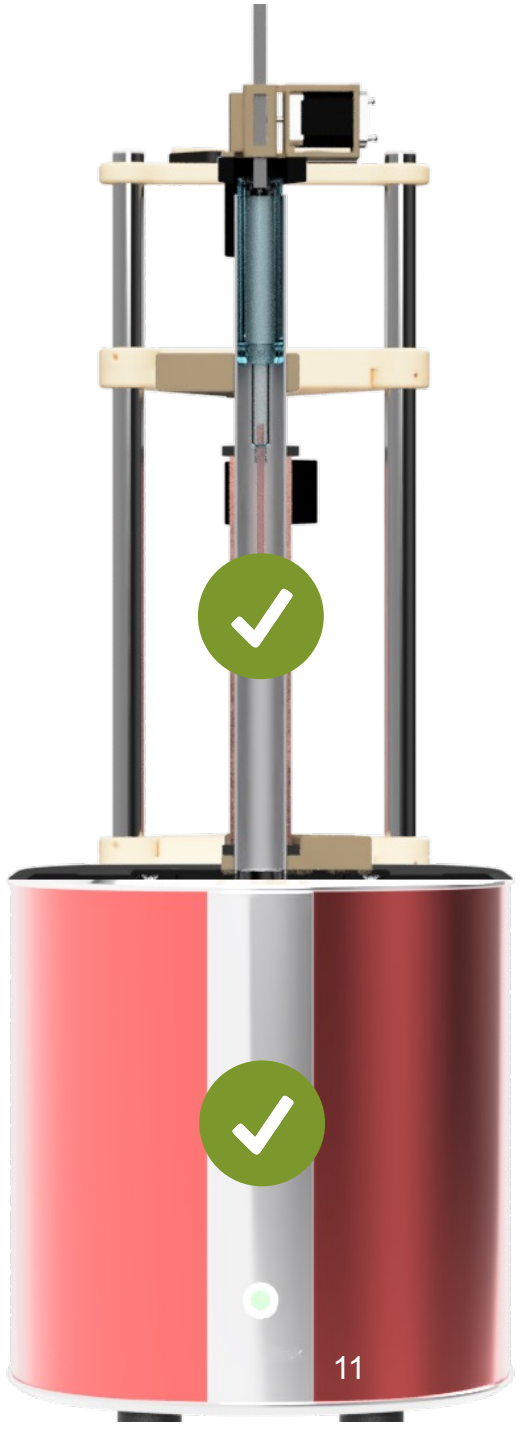


off-the-shelf part

3D-printed part

Low-cost magnetic field cycling system for benchtop NMR spectrometer

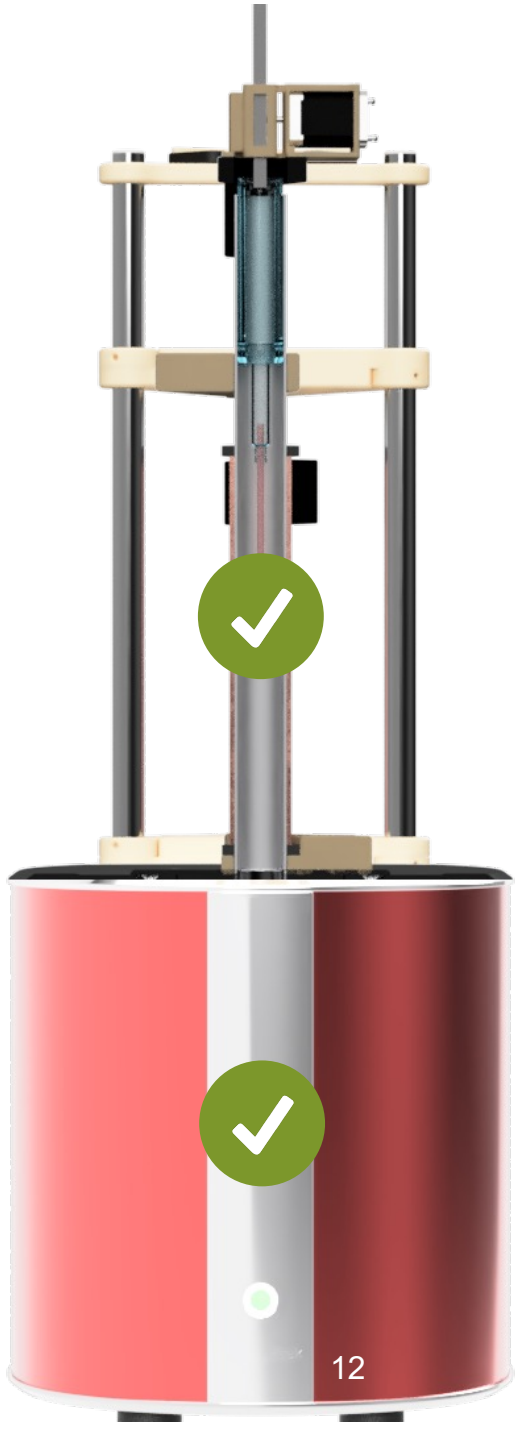
So what's missing to do PHIP?



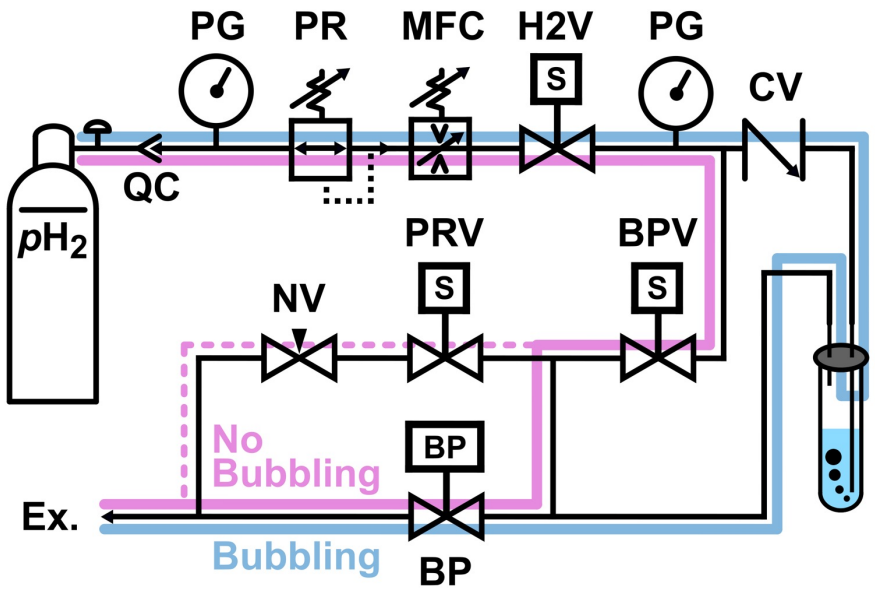
Low-cost magnetic field cycling system for benchtop NMR spectrometer

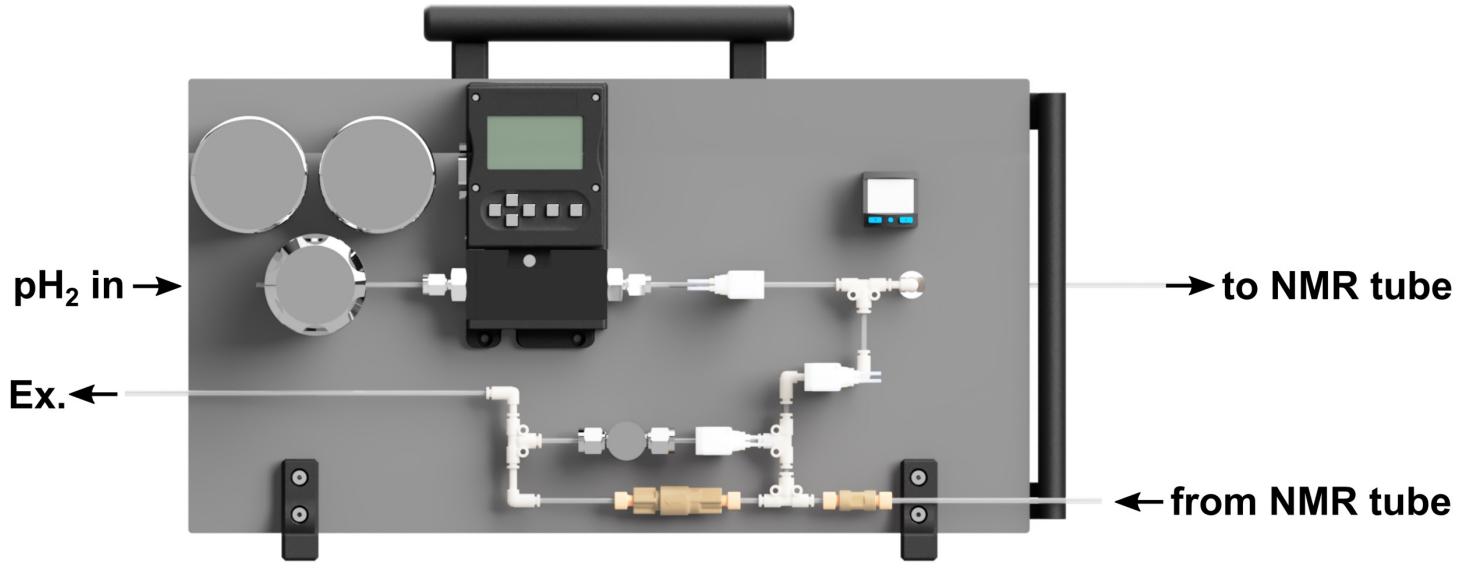
So what's missing to do PHIP?

- parahydrogen supply and reaction chamber



Add any bubbling setup!



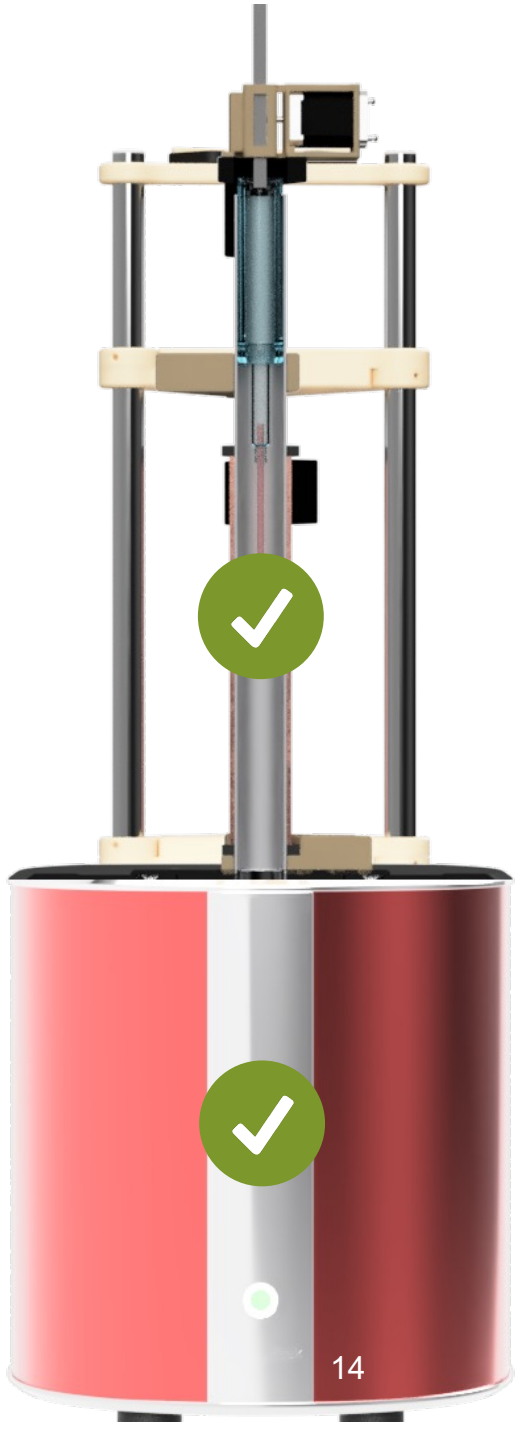


- Operated at **6.9 bar**
- Total cost **<4,200€**
- Controlled by ByteBoard

Low-cost magnetic field cycling system for benchtop NMR spectrometer

So what's missing to do PHIP?

- ✓ parahydrogen supply and reaction chamber

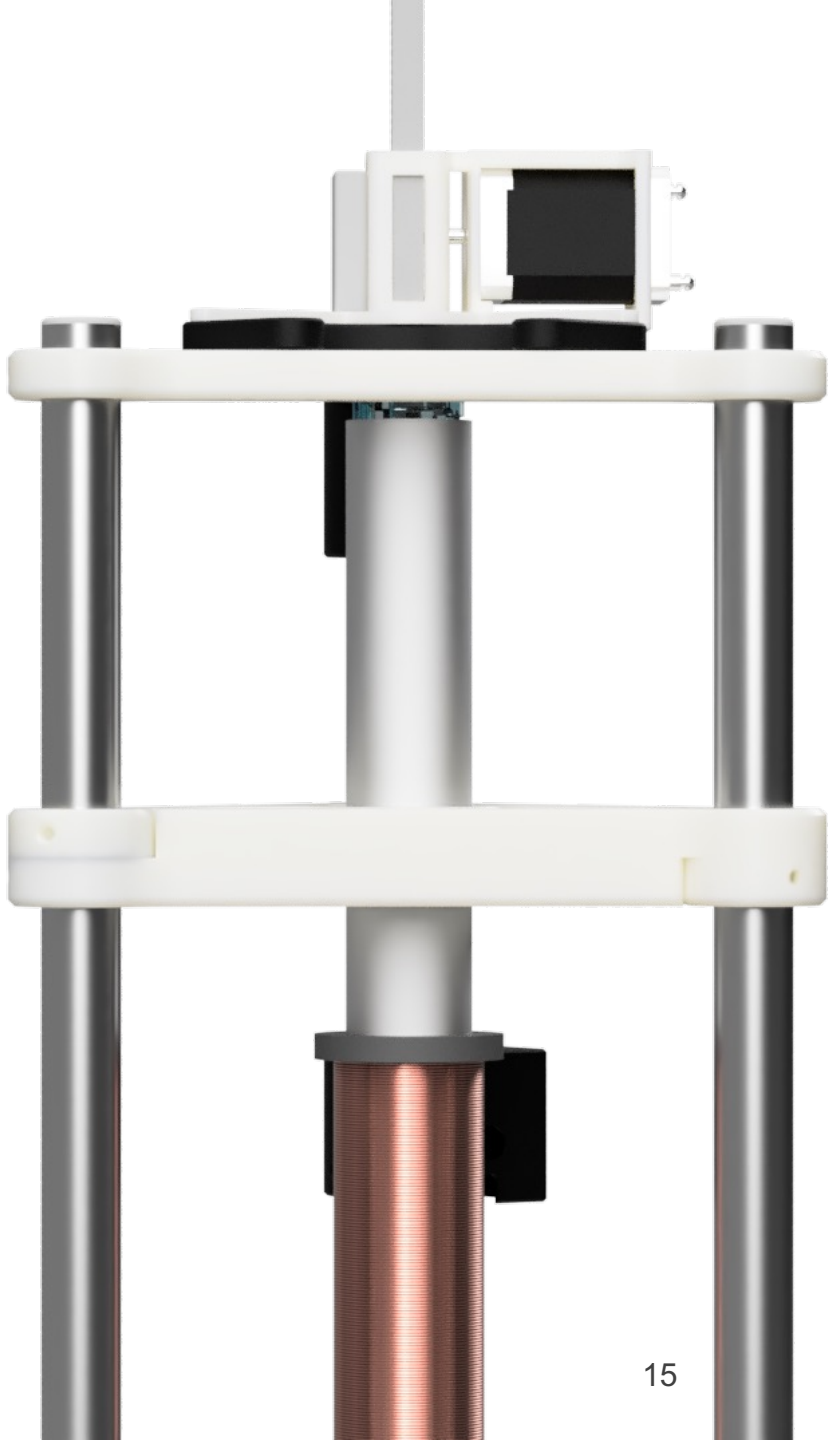


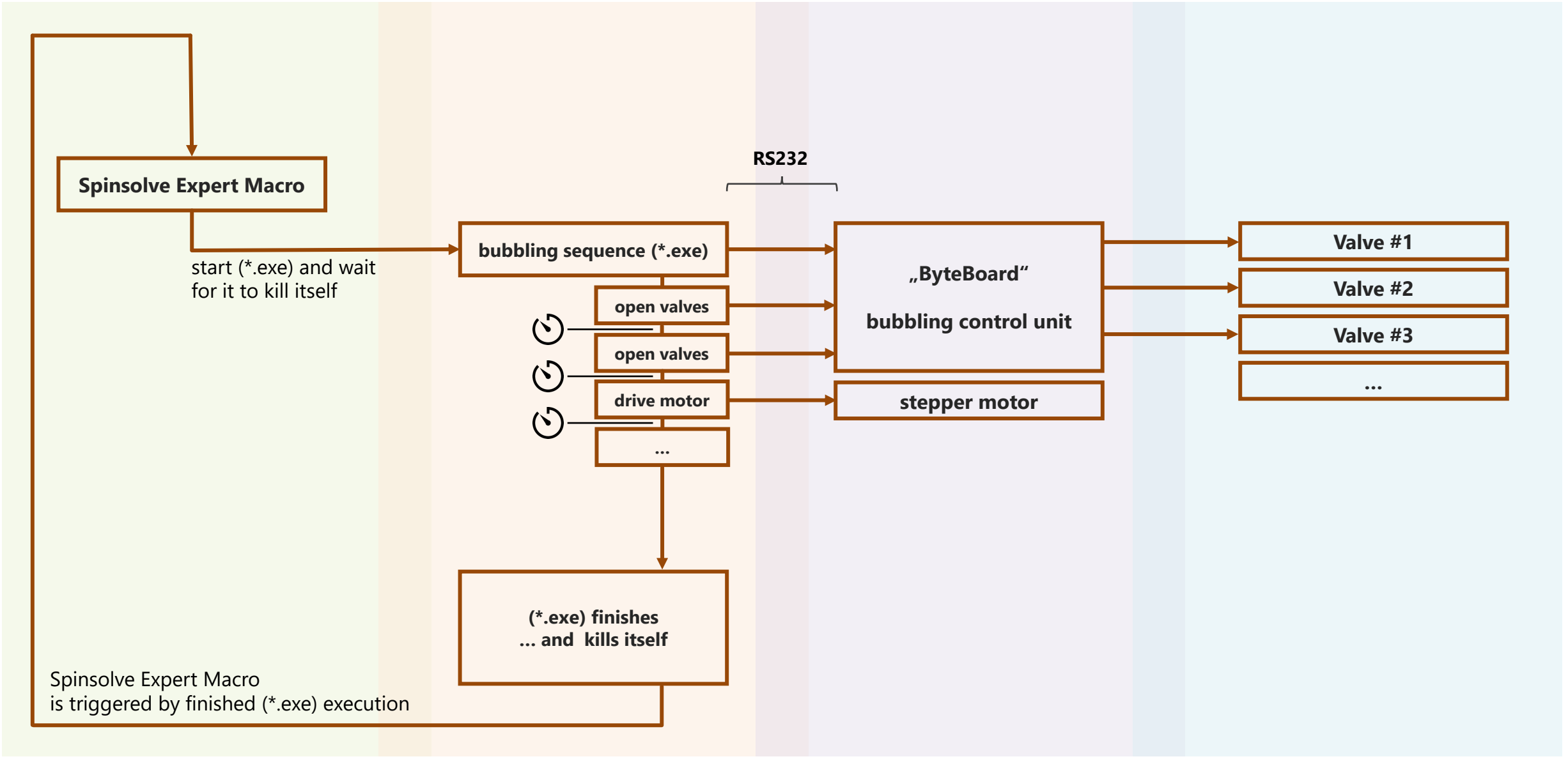
deconstruction of the title

about hardware

about software

about applications

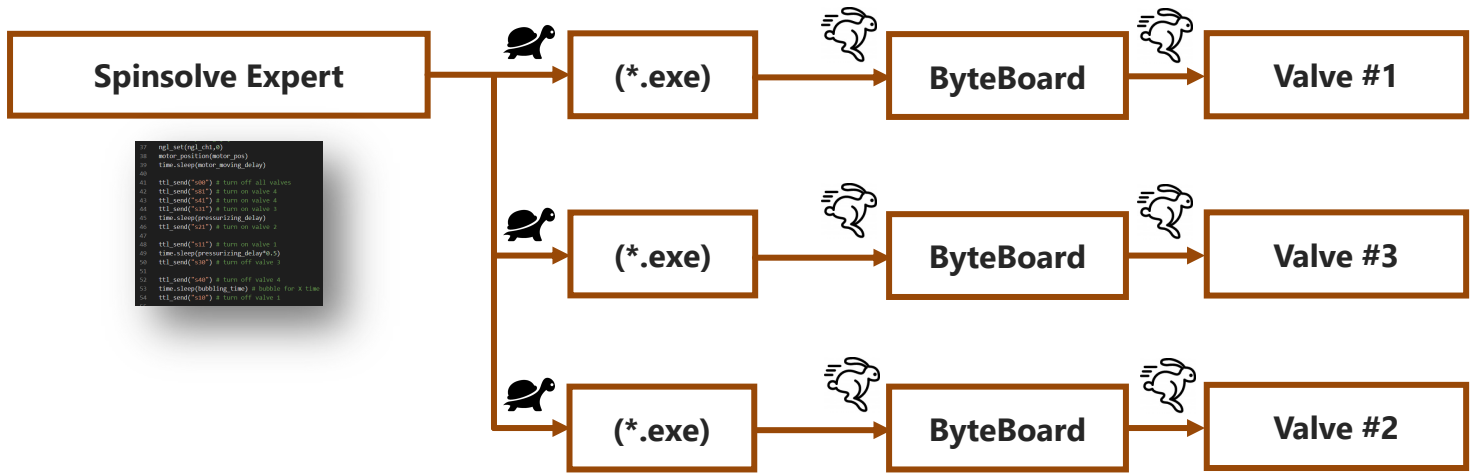



Spinsolve Expert
compiled Python script
Arduino or Motor
Valves
Spinsolve Expert Macro
start (*.exe) and wait
for it to kill itself
RS232
bubbling sequence (*.exe)
open valves
open valves
drive motor
...
„ByteBoard“
bubbling control unit
stepper motor
Valve #1
Valve #2
Valve #3
...
(*.exe) finishes
... and kills itself
Spinsolve Expert Macro
is triggered by finished (*.exe) execution

Why so complicated?

Naive straightforward approach

200 ms for opening RS232 connection for every command

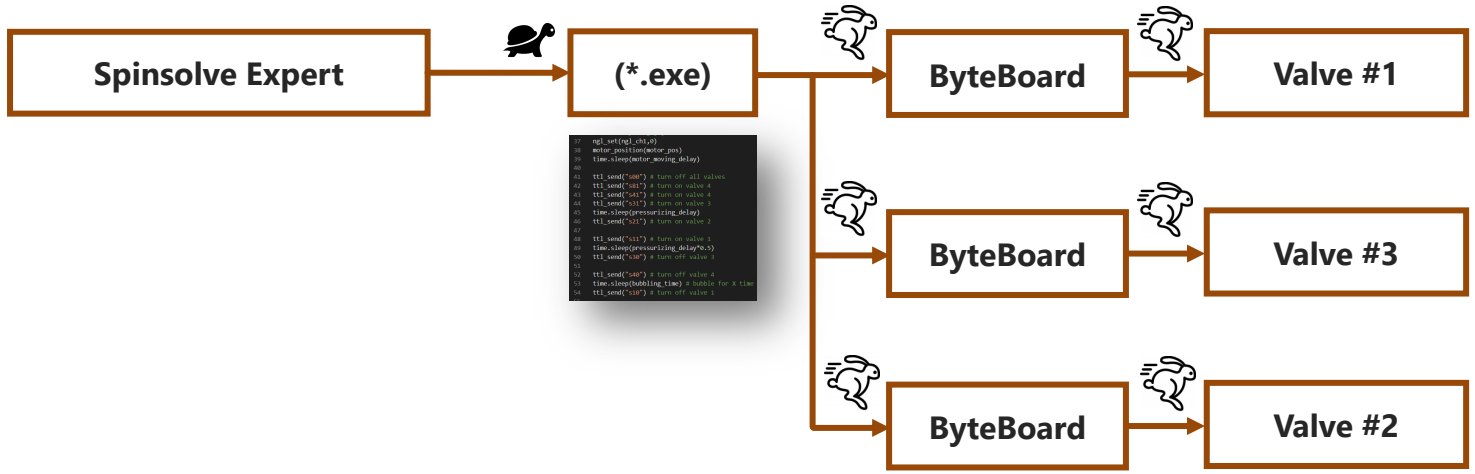


3x for 3 commands

Why so complicated?

Our new approach

Move experiment code to a compiled (*.exe) file



1x **for 3 commands**

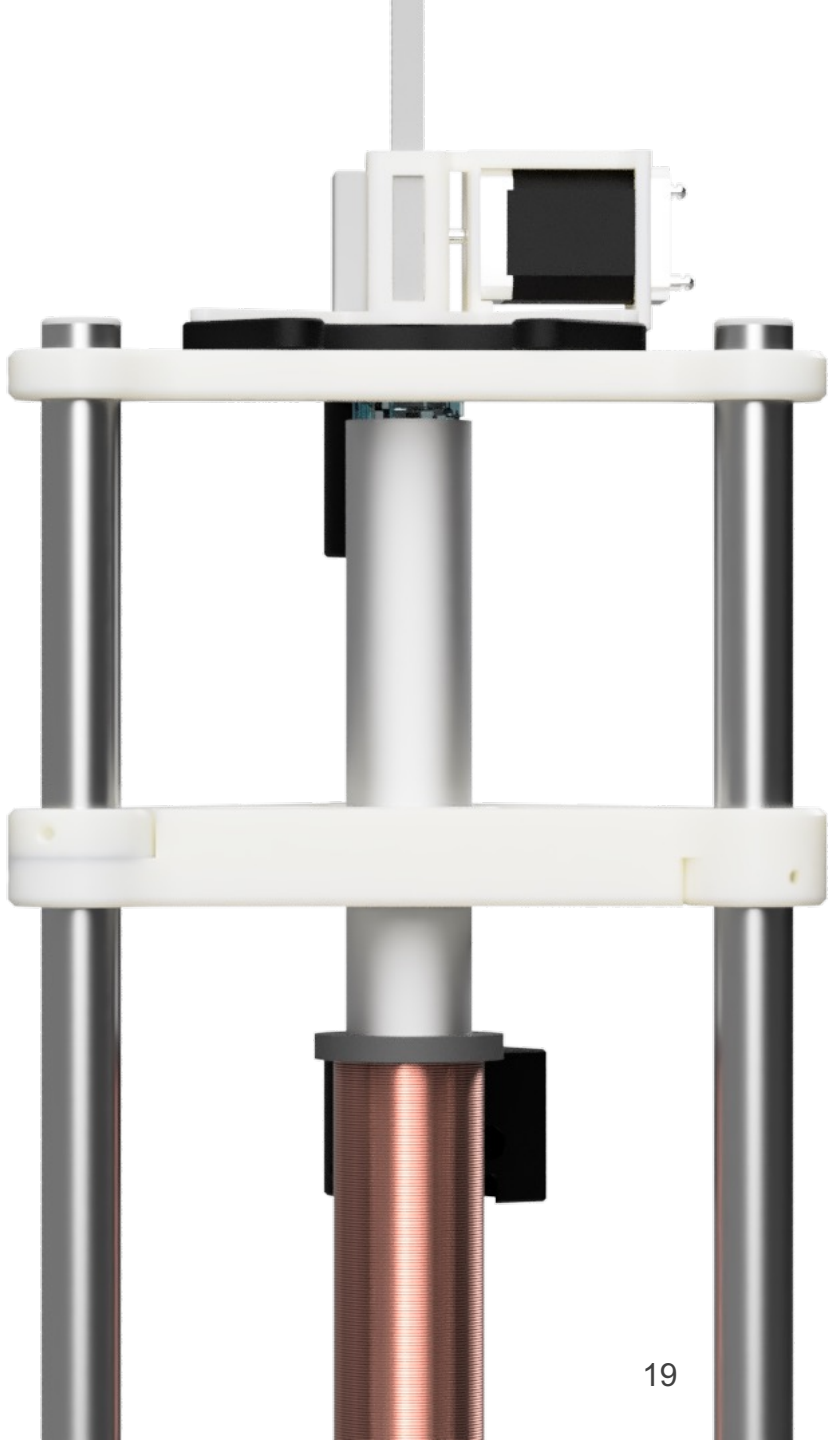
plus: the delay is before the actual experiment

deconstruction of the title

about hardware

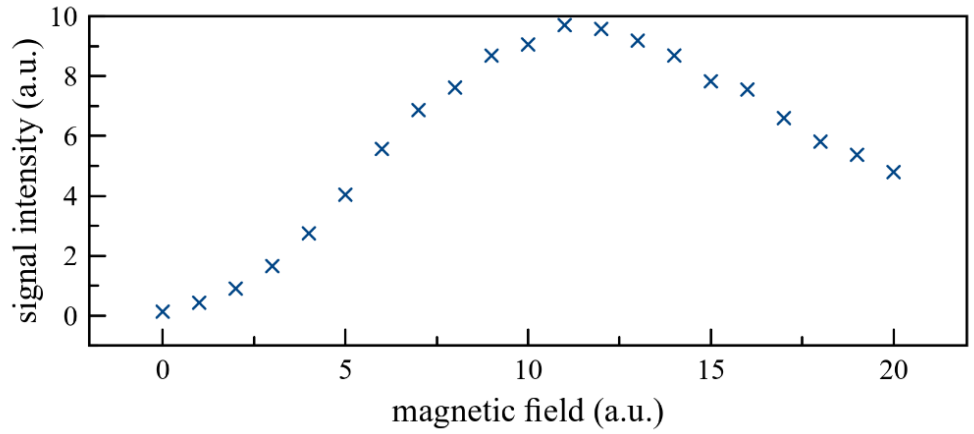
about software

about applications



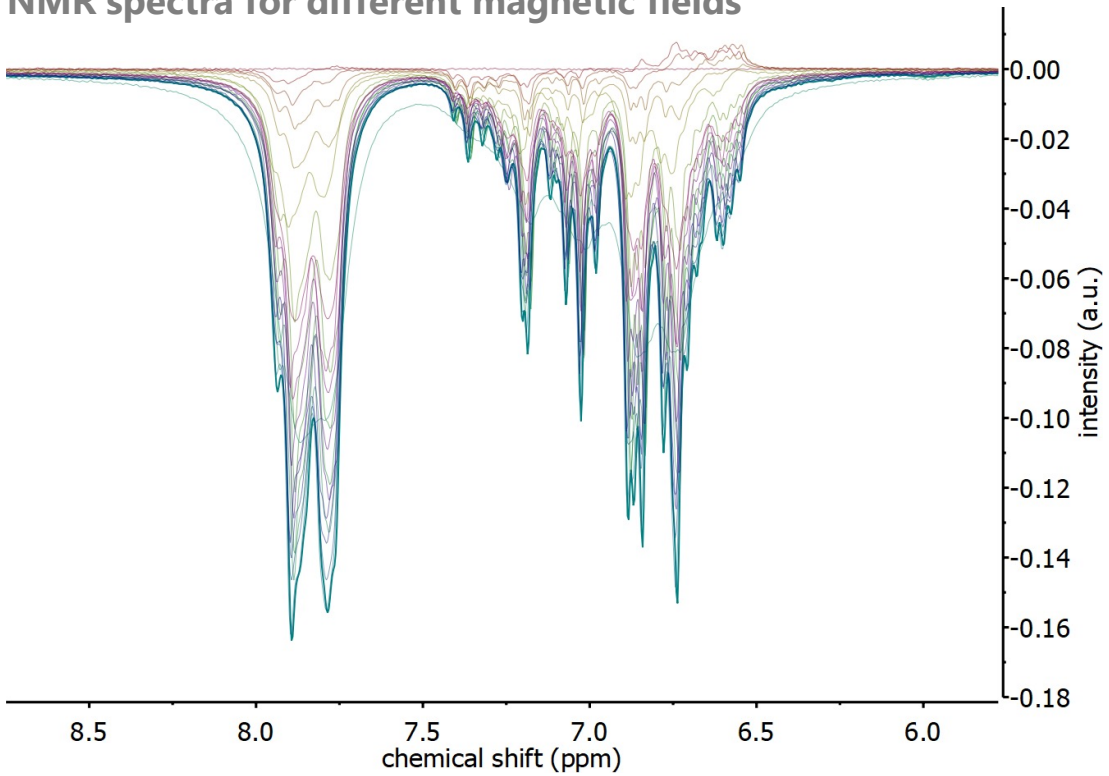
Hyperpolarization of pyridine with SABRE MFC

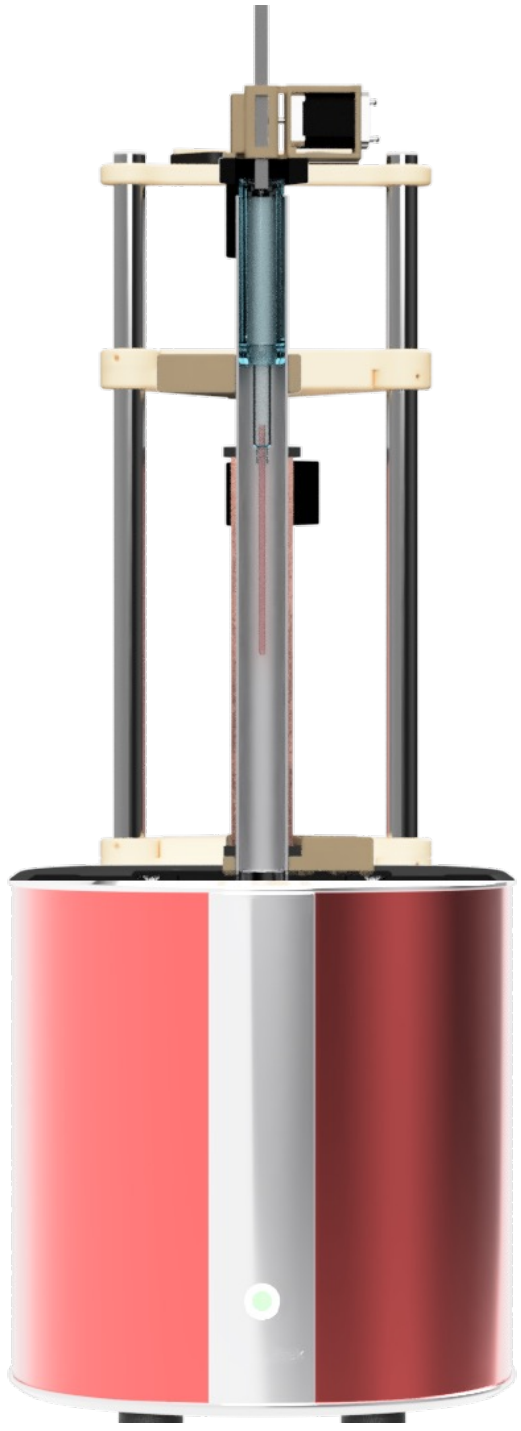
Signal intensity vs. magnetic field



(Peak integral of ortho-H in pyridine at different magnetic fields during hyperpolarization)

NMR spectra for different magnetic fields





Thank you!

SPECIAL THANKS TO MY SUPERVISORS
Dr. Andrey Pravdivtsev
Prof. Dr. Jan-Bernd Hövener

AND
Magritek for providing 3D-rendering of the Spinsolve spectrometer