
IOCB SERVICE DAYS

Presentation of services by:
Research-Service Groups / Service Groups / Core Facilities

20
23

Magnetic Resonance

Martin Dračínský



ÚOCHB AV
ČR
IOCB PRAGUE



NMR & EPR spectroscopy services

- Self-service NMR spectroscopy
- Advanced NMR spectroscopy
- EPR spectroscopy



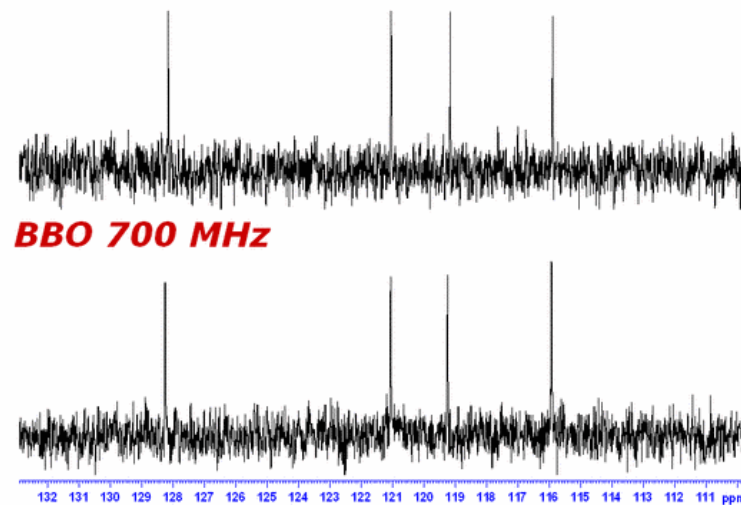
Self-service NMR measurements

- 2 × 400-MHz spectrometer, room A1.70b (NorthEast wing)



Prodigy 400 MHz

- Nitrogen-liquid cooled probes (PRODIGY)
2 × higher sensitivity



- More than **200 active users**
 - **Training** of new users every Monday at 9am
 - For registration, write an email to nmr-400@uochb.cas.cz
 - **Maintenance time** every Monday 9–11am
 - ^1H , ^{13}C , ^{19}F , ^{31}P and ^{11}B one-dimensional experiments
 - Basic 2D experiments (COSY, HSQC, HMBC)
 - Limitations: no variable-temperature experiments, no NOE experiments, no ^{15}N experiments
- The NMR self-service team:



Martin
Dračinský



Radek
Pohl



Ondřej
Socha



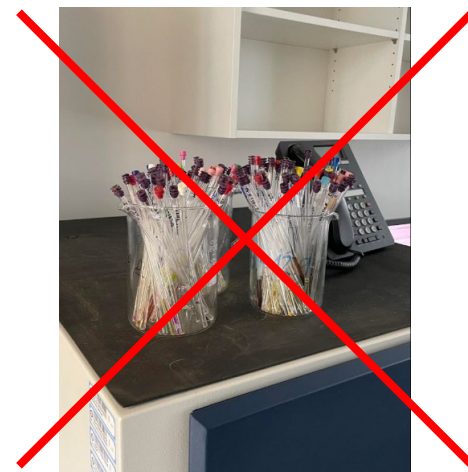
Jakub
Štoček



Serhii
Suikov

Self-service NMR measurements

- Write an email to nmr-400@uochb.cas.cz for “24/7” support
 - We have tools for remote access
- Email to all active users: nmr-users@uochb.cas.cz
- NMR tubes available in the storage of consumable supplies (B01.12)
- Deuterated solvents: chemical storage (B1.07)
- Always measure and check ^1H spectrum before submitting ^{13}C and 2D experiments
- Pick up your samples (over **100 samples per month** are **abandoned**)
- Do not leave tubes in rotor holders: high risk of sample damage, spillage and injury
- Keep the self-service lab **nice and tidy** for other users



- Measurement of samples with low-concentration
 - Cryoprobes
- NOE-based experiments
 - 3D structure
- Variable-temperature experiments
 - from -140 to $+140$ °C
- Other nuclei
 - ^2H , ^{15}N , ^{29}Si , ^{77}Se , ^{119}Sn , ^{125}Te and ^{195}Pt , ...
- Less common experiments
 - $^{13}\text{C}\{^1\text{H}, ^{19}\text{F}\}$; C,F-HMQC; C,F-HMBC; H,F-HOESY, H,N-HSQC; H,N-HMBC, ...
- Monitoring of reaction kinetics
 - observing one or more sensitive nuclei (^1H , ^{19}F , ^{31}P) at various temperatures
- In situ optical irradiation
 - irradiation by UV/vis light directly in the NMR tube
- Paramagnetic NMR
 - special setup and pulses sequences
- Solid-state NMR
 - probe for ultra-fast MAS, probe with extended temperature range (from -100 to $+200$ °C). ^1H and ^{19}F spectra with high resolution, H-C, H-P, H-N correlation, ...

NMR Spectroscopy - equipment

- Helium-gas cooled probes
 - 4–5 × higher sensitivity
 - Expensive
 - Regular maintenance necessary
- NMR spectrometers with cryoprobes: 1 × 600-MHz and 1 × 500-MHz spectrometer
 - 1.7-mm cryoprobe on 600-MHz spectrometer for the ultimate sensitivity



NMR Spectroscopy - equipment

- Versatile NMR spectrometers: 2 × 500-MHz spectrometer (temperature, F decoupling, other nuclei)

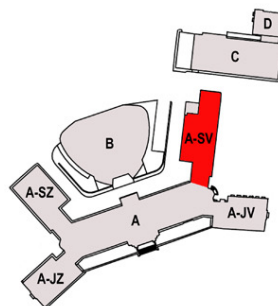


- Solid-state NMR: 1 × 600-MHz



NMR Spectroscopy Group - Contacts

- Building A1 – NorthEast wing



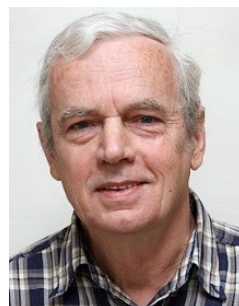
- NMR senior staff



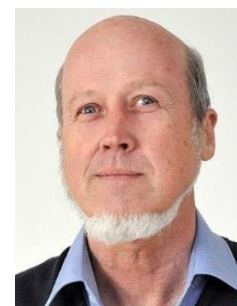
Martin
Dračínský



Radek
Pohl



Miloš
Buděšínský



David
Šaman
(emeritus)



Lenka
Poštová Slavětínská



Eliška
Procházková



Jan
Blahut



Serhii
Suikov

- technique for characterization of paramagnetic species (radicals, coordination metal complexes, defects in solid-state structures)
- EPR may provide:
 - chemical structure of the unpaired e^- center
 - concentration/number of paramagnetic species in the sample.
 - detection limit $\approx 10^{-7}$ – 10^{-8} mol dm $^{-3}$
- Advanced methods:
 - in situ UV/vis irradiation
 - combination of EPR with electrochemistry
 - spin trapping
 - ENDOR
- EPR contact



Ján Tarábek

- EPR spectrometer at IOCB (9.8 GHz, CW mode)



Try our NMR Challenge!

➤ nmr-challenge.com

- Solve structures of unknown compounds from NMR spectra
- 1D and 2D NMR spectra



NMR CHALLENGE
IOCB Prague



Basic ➤ Easy ➤ 2



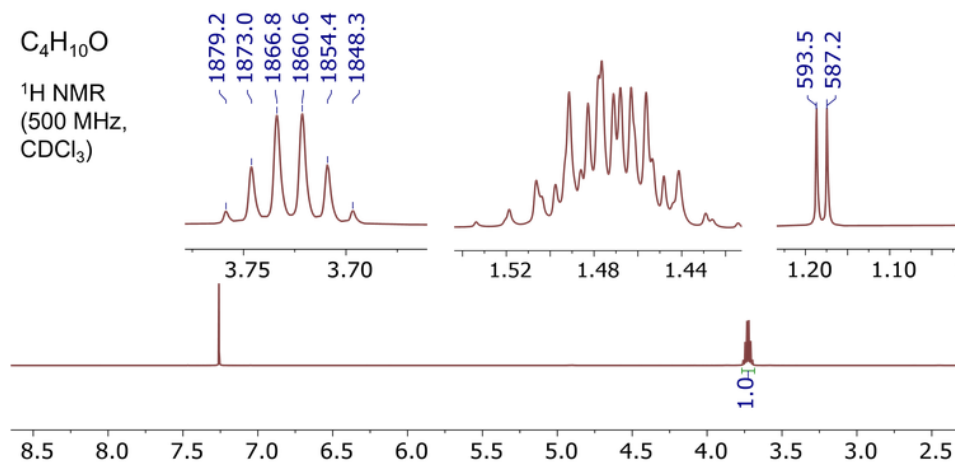
✓ Task 2 (Easy)

Next task »

Spectra

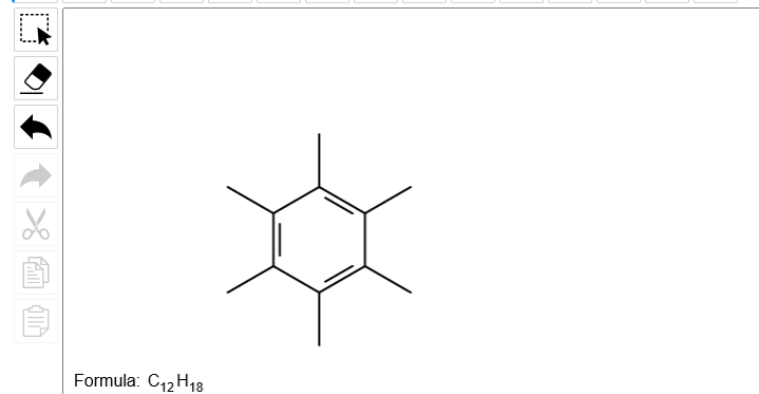
$C_4H_{10}O$

1H NMR
(500 MHz,
 $CDCl_3$)



Draw your solution

C N O S F Cl Br I + -    



Submit solution