# NMR@Empa: 400 MHz NMR Spectrometer (Bruker AV III HD 400 MHz widebore NMR spectrometer from 06-2014) with automation, HR-MAS and CP-MAS Utilities

Our 400 MHz NMR spectrometer is generally available for use directly by authorised people from the partner institutions Empa and Eawag. We also perform NMR measurements for external customers.



## **Spectrometer Hardware and Software:**

Our instrument is equipped with:

- actively shielded 400 MHz ASCEND<sup>TM</sup> superconducting magnet system with vibration damping
- two rf channels with BLAXH 300/100 amplifier for solution state applications
- BOSS shim system with 20 shim gradients
- digital <sup>2</sup>H lock control unit
- B-SVT digital temperature control system with BCU II unit for cooling down to -50°C
- B-SVT low temperature accessory for cooling with liquid nitrogen
- GRASP II unit for generation of z gradients

- automatic sample-changer unit (SampleCase, 24 position carousel)
- BLAH1000 and BLAX1000 linear high power transmitters for solid state applications
- fully automatic MAS pneumatic unit for spinning control of solid state NMR experiments
- the spectrometer is controlled by a Linux-PC running under TOPSPIN 3.x
- software upgrade for NUS processing
- CMC-se structure elucidation software

#### Frequently used NMR probes:

- 5 mm BBO CryoProbe<sup>™</sup> Prodigy with automatic tune and match (ATM); measuring temperature -40 to 80°C
- 2.5 mm CP-MAS BB ( ${}^{1}\text{H}/{}^{19}\text{F}$ ;  ${}^{15}\text{N}$   ${}^{31}\text{P}$ , 40.6 162.0 MHz), MAS rates up to 35 kHz, 15 µl effective sample volume; measuring temperature up to 70°C
- 4 mm CP-MAS BB (<sup>1</sup>H/<sup>19</sup>F; <sup>15</sup>N <sup>31</sup>P, 40.6 162.0 MHz), MAS rates up to 15 kHz, 80 μl effective sample volume; measuring temperature up to 120°C
- 7 mm CP-MAS BB ( ${}^{1}\text{H}/{}^{19}\text{F}$ ;  ${}^{15}\text{N}$   ${}^{31}\text{P}$ , 40.6 162.0 MHz), MAS rates up to 6 kHz, 300 µl effective sample volume; measuring temperature up to 120°C
- 4 mm HR-MAS (<sup>1</sup>H; <sup>13</sup>C), MAS rates up to 5 kHz, 15 or 50 μl effective sample volume; measuring temperature -20 to 80°C

## Less frequently used probes:

- 5 mm BB inverse (<sup>1</sup>H/<sup>19</sup>F; <sup>109</sup>Ag <sup>31</sup>P, 26.6 162.0 MHz) with an actively shielded z-gradient coil; measuring temperature -100 to 120°C
- 5 mm BB observe ( ${}^{1}\text{H}/{}^{19}\text{F}$ ;  ${}^{109}\text{Ag}$   ${}^{31}\text{P}$ , 26.6 162.0 MHz); measuring temperature -100 to 120°C
- 10 mm SEX ( $^{1}$ H;  $^{2}$ H with  $^{19}$ F lock)

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