

## Instructions for filling in the NMR request form

**Please fill out the request form digitally or write clearly in block letters! Please select short names with a maximum of ten characters for the sample description.**

All technical and scientific employees of the Department of Chemistry receive a department ID from the user administration of the IT Service. On the one hand, this is used for email service, e.g., but also to manage analytical data. Each employee is assigned to an institute and a working group. Students can receive the department ID at the latest from the Master's thesis onwards if they are assigned to a working group. The department ID is your login name for the email server (@chemie.uni-hamburg.de).

Depending on the type of sample/order there are different request forms (e.g. standard sample, lab course, temperature measurement, etc.): <https://www.chemie.uni-hamburg.de/en/service/wissenschaftlicher-service/nmr/service.html>.

ABOUT THE DEPARTMENT

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INSTITUTES

PEOPLE

SERVICE



### SUBMISSION OF NMR SAMPLES

The NMR facility is a central facility and is open to all users of the department of chemistry. Users are members of scientific working groups or students who carry out NMR measurements during lab courses. External measurements can be carried out on request to the scientific heads of the NMR department. Costs for such measurements can also be requested.

Below you will find our request forms and information on the measurements. Please use only the current request forms!

#### General information:

- The length of the tubes (5 mm and 10 mm) must be at least 16.5 cm and at most 18 cm.
- The filling height must not be less than 4.5 cm and should not be more than 6 cm.
- Deuterated solvents must be used (enter on the request form).
- The sample must be completely dissolved, so that the solution is homogeneous liquid with low viscosity.
- In general, you should give as much sample as you can. Doubling the sample quantity reduces the measuring time by a factor of 4!
- [Further instructions for filling out the request forms](#)

Please remember to pick up measured NMR samples immediately! The samples are sorted according to the working groups, so that the samples of other group members can be taken along. NMR samples that have not been collected are disposed of at regular intervals!

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+ Open Access Spectrometer

+ Measurements at Different Temperatures

+ Solid State NMR

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Save the corresponding request form and open it. When you open it for the first time, the document (standard and polymer samples) will look like this:

<p>Standard sample - phone: [ ] date: [ ] Institute - working group - name (Department ID) IAC - (AC) - [ ] sample description (max. 12 characters): [ ] special measurement: <input type="checkbox"/> 600 MHz <input type="checkbox"/> other: [ ] solvent: [ ] amount: [ mg ] Mol-mass (ca.): [ g/mol ] 1D-Standard: <input type="checkbox"/> <sup>1</sup>H <input type="checkbox"/> <sup>31</sup>P{H}-BB <input type="checkbox"/> <sup>19</sup>F <input type="checkbox"/> <sup>1</sup>H is measured and approved! ----- <input type="checkbox"/> <sup>13</sup>C-DEPTQ <input type="checkbox"/> <sup>13</sup>C{H}-BB 2D-Standard: <input type="checkbox"/> COSY <input type="checkbox"/> HSQC <input type="checkbox"/> HMBC <input type="checkbox"/> TOCSY <input type="checkbox"/> NOESY measurement range for <sup>31</sup>P/<sup>19</sup>F: [ ] ppm automation number: possible comments on the back</p>	<p>Standard sample - phone: [ ] date: [ ] Institute - working group - name (Department ID) IAC - (AC) - [ ] sample description (max. 12 characters): [ ] special measurement: <input type="checkbox"/> 600 MHz <input type="checkbox"/> other: [ ] solvent: [ ] amount: [ mg ] Mol-mass (ca.): [ g/mol ] 1D-Standard: <input type="checkbox"/> <sup>1</sup>H <input type="checkbox"/> <sup>31</sup>P{H}-BB <input type="checkbox"/> <sup>19</sup>F <input type="checkbox"/> <sup>1</sup>H is measured and approved! ----- <input type="checkbox"/> <sup>13</sup>C-DEPTQ <input type="checkbox"/> <sup>13</sup>C{H}-BB 2D-Standard: <input type="checkbox"/> COSY <input type="checkbox"/> HSQC <input type="checkbox"/> HMBC <input type="checkbox"/> TOCSY <input type="checkbox"/> NOESY measurement range for <sup>31</sup>P/<sup>19</sup>F: [ ] ppm automation number: possible comments on the back</p>
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Select your institute and the working group to which you belong from the list. The changes you make in the two fields always affect all four forms simultaneously.

The image displays four identical screenshots of a data entry form, arranged in a 2x2 grid. Each form contains the following fields and options:

- Standard sample -
- phone: [input field]
- date: [input field]
- Institute - working group - name (Department ID): IOC - HACK - [input field]
- sample description (max. 12 characters): [input field]
- special measurement:  600 MHz  other: [input field]
- solvent: [input field] amount: [input field] mg Mol-mass (ca.): [input field] g/mol
- 1D-Standard:  <sup>1</sup>H  <sup>31</sup>P{H}-BB  <sup>19</sup>F
- <sup>1</sup>H is measured and approved!
- <sup>13</sup>C-DEPTQ  <sup>13</sup>C{H}-BB
- 2D-Standard:  COSY  HSQC  HMBC  TOCSY  NOESY
- measurement range for <sup>31</sup>P/<sup>19</sup>F: [input field] ppm
- automation number:
- possible comments on the back

Red boxes highlight the 'IOC' and 'HACK' dropdown menus in all four screenshots, indicating that these selections are shared across all forms.

Furthermore, the document "remembers" the entry Institute and working group, regardless of whether you save the document. This means that you do not have to re-enter the two fields each time.

Now enter your Department ID in the Name field (Department ID). The name is automatically entered in all four forms of the document. The same applies to the telephone number. Please always include the telephone number so that we can contact you if we have any questions.

<p>Standard sample . phone: <input type="text"/> date: <input type="text"/></p> <p>Institute - working group - name (Department ID)</p> <p>IOC . - HACK . - doe</p> <p>sample description (max. 12 characters): <input type="text"/></p> <p>special measurement: <input type="checkbox"/> 600 MHz <input type="checkbox"/> other: <input type="text"/></p> <p>solvent: <input type="text"/> amount: <input type="text"/> mg Mol-mass (ca.): <input type="text"/> g/mol</p> <p>1D-Standard: <input type="checkbox"/> <sup>1</sup>H <input type="checkbox"/> <sup>31</sup>P{H}-BB <input type="checkbox"/> <sup>19</sup>F  <input type="checkbox"/> <sup>1</sup>H is measured and approved!</p> <p><input type="checkbox"/> <sup>13</sup>C-DEPTQ <input type="checkbox"/> <sup>13</sup>C{H}-BB</p> <p>2D-Standard: <input type="checkbox"/> COSY <input type="checkbox"/> HSQC <input type="checkbox"/> HMBC <input type="checkbox"/> TOCSY <input type="checkbox"/> NOESY</p> <p>measurement range for <sup>31</sup>P/<sup>19</sup>F: <input type="text"/> ppm</p> <p>automation number:</p> <p>possible comments on the back</p>	<p>Standard sample . phone: <input type="text"/> date: <input type="text"/></p> <p>Institute - working group - name (Department ID)</p> <p>IOC . - HACK . - doe</p> <p>sample description (max. 12 characters): <input type="text"/></p> <p>special measurement: <input type="checkbox"/> 600 MHz <input type="checkbox"/> other: <input type="text"/></p> <p>solvent: <input type="text"/> amount: <input type="text"/> mg Mol-mass (ca.): <input type="text"/> g/mol</p> <p>1D-Standard: <input type="checkbox"/> <sup>1</sup>H <input type="checkbox"/> <sup>31</sup>P{H}-BB <input type="checkbox"/> <sup>19</sup>F  <input type="checkbox"/> <sup>1</sup>H is measured and approved!</p> <p><input type="checkbox"/> <sup>13</sup>C-DEPTQ <input type="checkbox"/> <sup>13</sup>C{H}-BB</p> <p>2D-Standard: <input type="checkbox"/> COSY <input type="checkbox"/> HSQC <input type="checkbox"/> HMBC <input type="checkbox"/> TOCSY <input type="checkbox"/> NOESY</p> <p>measurement range for <sup>31</sup>P/<sup>19</sup>F: <input type="text"/> ppm</p> <p>automation number:</p> <p>possible comments on the back</p>
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All other entries such as date, sample name or selection of experiments are only made on the request form processed in each case.

Under other you can select whether the sample is sensitive to light or air, or whether a paramagnetic sample is submitted. For paramagnetic samples, please specify the desired measuring range. Other special features of the sample can also be entered manually in the field. Further information about the sample or the measurement can be noted on the back.

Please note that for measurements of time-consuming 1D-<sup>13</sup>C and 2D experiments require the measurement of a simple <sup>1</sup>H-NMR experiment in advance for (self-)control purposes.

Standard sample ▾ phone:  date:   
Institute - working group - name (Department ID)  
IOC ▾ - HACK ▾ - doe   
sample description (max. 12 characters):   
special measurement:  600 MHz  other:   
solvent:  amount:  mg Mol-mass (ca.):  g/mol  
1D-Standard:  <sup>1</sup>H  <sup>31</sup>P{H}-BB  <sup>19</sup>F  
 <sup>1</sup>H is measured and approved!  

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 <sup>13</sup>C-DEPTQ  <sup>13</sup>C{H}-BB  
2D-Standard:  COSY  HSQC  HMBC  TOCSY  NOESY  
measurement range for <sup>31</sup>P/<sup>19</sup>F:  ppm  
automation number:  
possible comments on the back

Please also pay attention to the legibility of the NMR request form and use them only twice for sample submission!

### Special instructions of Open Access measurements

Please fill out a separate form for each NMR sample so that it is possible to assign the samples. Please fill in the document completely as with all other request forms. The telephone number is important for a quick contact in case of questions or other problems!

**Please always enter the sample position in the field provided.** The sample position must match the entry in ICON-NMR and the actual position in the sampler.

OpenAccess	phone: 1234	date: 25.2.2020
Institute - working group - name (Department ID)		
SER	- NMRS	- doe
sample description (max. 12 characters): doe's sample		
solvent: CDCl <sub>3</sub>	amount: 123 mg	Mol-mass (ca.): 123 g/mol
Sample position:	<input type="text" value="08"/>	
comment:	<input type="text"/>	

### **Special instructions for lab courses**

NMR samples can be measured within the following lab courses:

Basic lab course in Organic Chemistry (CHE 013)

Selection for institute-AK: PRA-OCP2-"NAME"

Chemistry including analysis of organic pharmaceuticals, excipients and pollutants (CHE 313B)

Selection for Institut-AK: PRA-PHA3-"NAME"

Integrated lab course on synthesis (CHE 020)

Selection for institute-AK: PRA-ISP5-"NAME"

Lab course for chemistry as secondary subject (CHE 061)

Selection for institute-AK: PRA-INFP-"NAME"

Since there is no department ID for students in the lab courses, please enter your surname under "NAME". Your assistants will help you to download the spectra from the server.