X.Y.Z Nuclear Magnetic Resonance (NMR)
(C. Farès – 8.6 FTE)

The NMR department provides a broad range of specialized NMR techniques and analytical service. During the reporting period, approximately 74,000 NMR spectra have been recorded on a wide range of samples, from natural products, active enzymes and metal complexes in solution to porous silicas and zeolites in solids. To meet demands, the department is equipped with six NMR spectrometers with field strengths corresponding to ^{1}H frequencies of 300, 400, 500 and 600 MHz for analyses in solution and of 300 and 500 MHz for analyses in solid state. The department is organised in three broad areas of service.

(1) Open-Access and Routine NMR: Scientific employee can carry out basic NMR measurements in liquid state in high-throughput mode on a dedicated “open access” 300-MHz NMR spectrometer. The selection of available experiments is limited to those with high sensitivity, high information content and rapid execution with predefined parameters. Liquid samples requiring special set-up or treatment can be submitted for measurement to our operators on available spectrometers. The most common requests are: (a) special nuclei, (b) high or low temperature NMR, (c) optimized experiments (eg. NOESYs), and (d) kinetic NMR chemical reactions. These services cover nearly 90% of all experiments run in our department.

(2) Advanced NMR: Particularly challenging NMR studies of solution compounds are accepted for advanced analysis. For these samples, our experienced staff members provide full measurement, analysis and interpretation assistance in close collaboration with the chemical research groups. The advanced techniques are carried out on dedicated spectrometer: (a) a high-sensitivity 600-MHz system, equipped with a cryogenically-cooled probehead, which is ideally suited for sub-milligram quantities of 50+ carbon organic molecules; (b) a more versatile modern 500-MHz instruments which provides the possibility to measure at high and low temperature, to cover a broad range of NMR-active isotopes, and to run advanced triple-resonance experiments. A large part of the analytical work is dedicated to determine or confirm structures, stereochemistries, conformations and dynamics.

(3) Solid-State NMR: Solid-state NMR spectroscopy remains one of the most important techniques for the characterisation of solid catalysts, functional materials and potential hydrogen storage materials synthesized in the institute (Schüth group). In continuation of work performed in previous years, solid-state NMR spectroscopy has particularly been applied for the characterisation of the following solids: (a) Catalysts and functional materials from mesoporous silicas or zeolites (^{29}Si, ^{13}C and ^{27}Al); (b) Complex aluminium hydrides (mainly ^{27}Al NMR); (c) Adducts of alane (AlH_3) with tertiary amines (^{13}C and ^{27}Al NMR); (d) Materials obtained by ball milling.

List of Talks Given by Members of the Institute

Farès, C.

- ORCA Summer School, Gelsenkirchen, DE, Sept. 2017
- Treffen der Junganalytiker der GDCh, Mülheim an der Ruhr, DE, Nov. 2017
- 40th Ann. Disc. Meeting FGMR/GDCh, Leipzig, DE, Sept. 2018

Special Events and Activities

Farès, C.

- Girlsday 2017, Mülheim/Ruhr, Apr. 2017
- Chemistry Show for Kindergarten Arche, Mülheim/Ruhr, Jun. 2017
- NMR Practical Training for Apprentices, Mülheim/Ruhr, Sep. 2017
- Optics Lecture for Physics Apprentices, Mülheim/Ruhr, Sep.-Dec 2017
- Girlsday 2018, Mülheim/Ruhr, Apr. 2018
- NMR Practical Training for Apprentices, Mülheim/Ruhr, Sep. 2018
- NMR Experimental Project with Pupils from Luisenschule, Mülheim, Jun. 2019
- Optics Lecture for Physics Apprentices, Mülheim/Ruhr, Sep.-Dec. 2019
- Course: NMR in Catalysis, IMPRS-RECHARGE, Mülheim/Ruhr, Nov. 2019

Leutzsch, M.

- Girlsday 2019, Mülheim/Ruhr, Apr. 2019
- NMR Practical Training for Apprentices, Mülheim/Ruhr, Sep. 2019

Farès

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