X-PULSE 90

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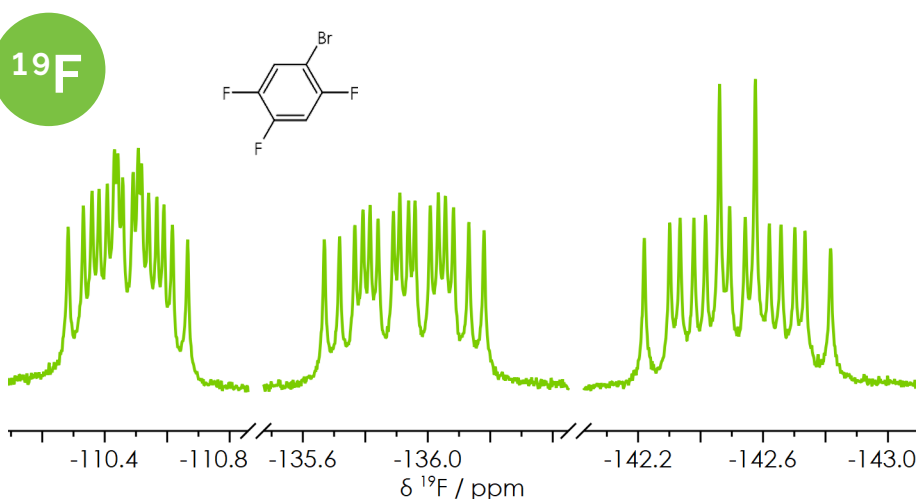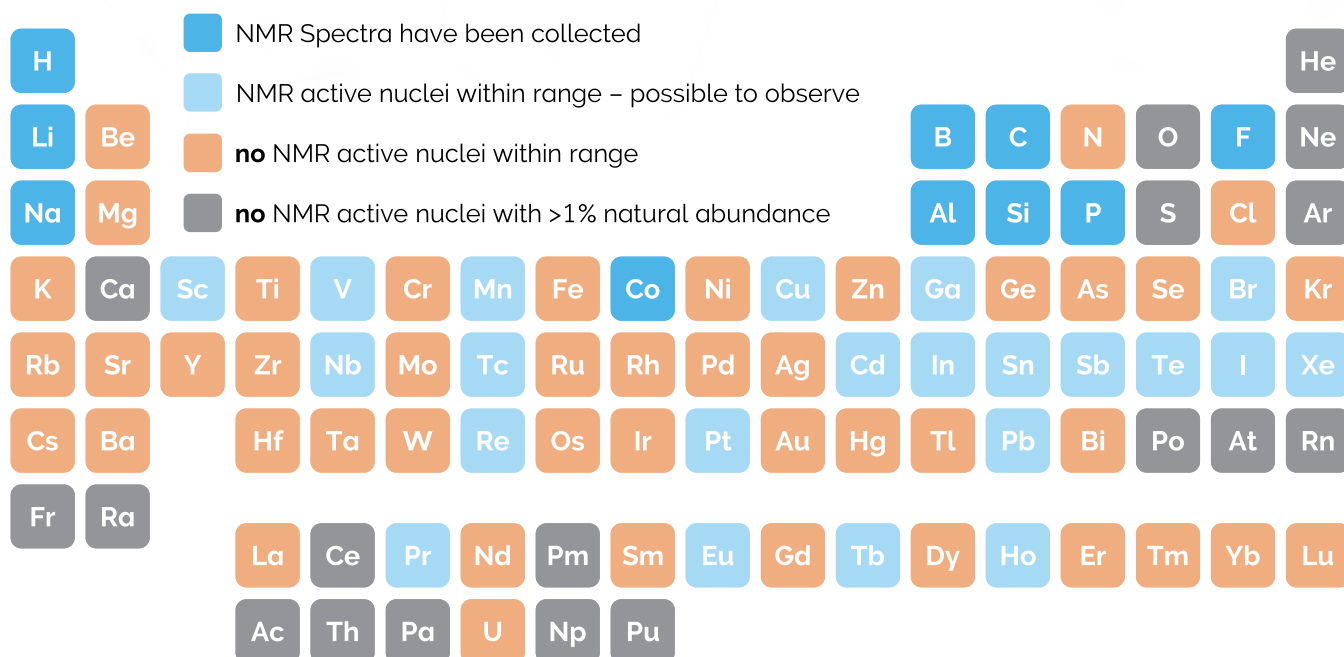## Broadband NMR Spectroscopy at 90 MHz on the Benchtop

Introducing the X-Pulse 90

X-Pulse 90 is a revolutionary new benchtop nuclear magnetic resonance (NMR) spectrometer that brings broadband NMR to the benchtop at 90 MHz for the first time. X-Pulse 90 is the ideal instrument for flexible chemical analysis, across a wide variety of applications, as it enables investigation of the largest number of nuclei without compromising performance.
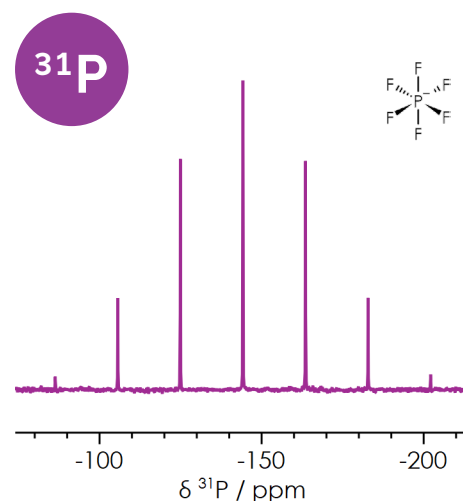
X-Pulse 90 continues the X-Pulse ethos of modularity, versatility, and upgradeability, and as such can be tailored to your needs, for example, with a flow cell to monitor real-time reactions, or the addition of variable temperature capability. Additionally, the unique, user exchangeable probe enables the setup to be easily changed depending on the requirements (e.g. highest signal to noise (SNR) performance versus multiple nuclei), as well as ease of access for cleaning.

X-Pulse's unique features that will benefit your workflow:

- Broadband capability enables a large number of nuclei to be measured

- A wide variable temperature range option of 0-60°C allowing users to thoroughly investigate reaction kinetics or characterise electrolyte properties

- The orientation of the diffusion gradient ensures accurate measurement, even in flow experiments

- User exchangeable probes mean no compromise between versatility and sensitivity

- User removeable probe means minimal machine downtime for breakages and spills

- NMR Spectra have been collected
- NMR active nuclei within range – possible to observe
- **no** NMR active nuclei within range
- **no** NMR active nuclei with >1% natural abundance

^{19}F spectrum of 1-bromo-2,4,5-trifluorobenzene

^{31}P spectrum of hexafluorophosphate

The Power of 90 MHz Performance

With a magnetic field of 90 MHz (2.1 T) X-Pulse 90 allows users to separate challenging peak overlaps and positively identify compounds of interest in samples. The increased spectral dispersion means that a peak that is hard to distinguish with a lower magnetic field is now separated and easily identifiable.

The increased sensitivity of X-Pulse 90 also enables detection and accurate measurement of molecules with a lower concentration, such as mass limited samples or when dealing with active pharmaceutical ingredients (APIs). The increased sensitivity and peak separation also enable much faster 2D experiments, even on larger molecules.
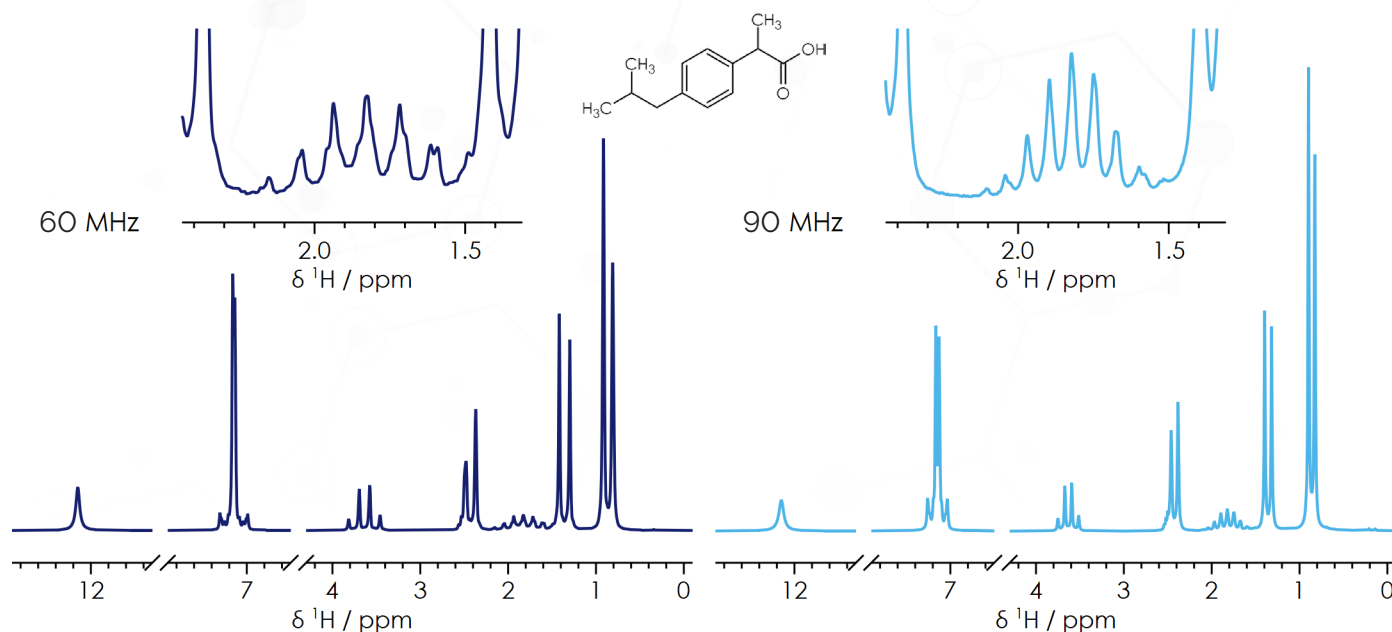
A comparison of ibuprofen ^{1}H spectroscopy on X-Pulse (60 MHz, left) and X-Pulse 90 (90 MHz, right). The zoomed in section highlights the better peak separation due to the higher field.
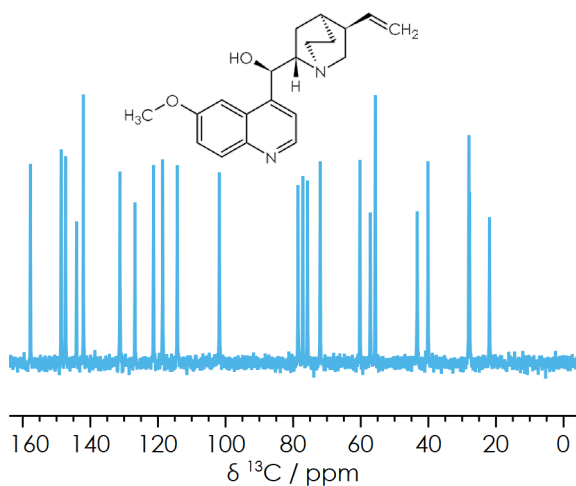
^{13}C{^{1}H} Spectrum of Quinine
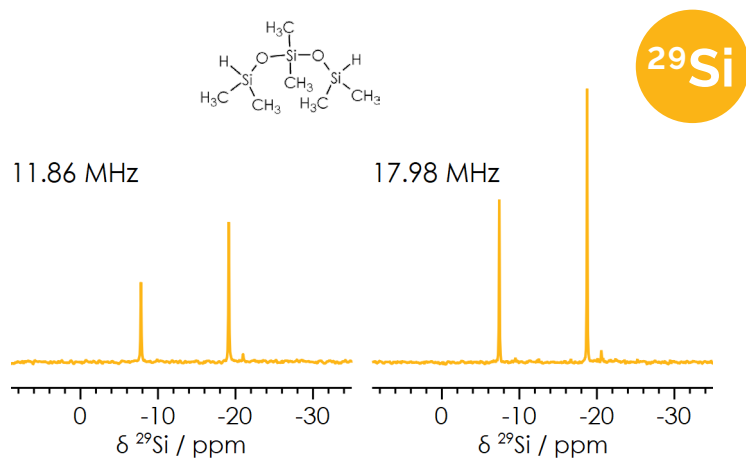
^{29}Si{^{1}H} spectra at 60 Mhz (left) and 90 MHz (right) the gain in SNR means more signal in less time on X-Pulse 90

Why Benchtop NMR Spectroscopy?

Benchtop NMR is a spectroscopic technique that provides structural and quantitative insights into liquid chemical samples. The minimal sample prep and non-invasive, non-destructive nature make it perfect for complementing any existing analysis techniques. Benchtop NMR can easily be brought to the lab, and when coupled with a flow cell and X-Pulse broadband capabilities, provides real time monitoring of many nuclei within a sample.

To speed up analysis, X-Pulse 90 can be fitted with a 25 position autosampler allowing 'hands free' analysis that reduces time spent in front of the instrument and maximises instrument use.

X-Pulse 90: Example Applications

X-Pulse 90 has applications in a wide variety of academic and industrial sectors:

- Pharmaceuticals – identify and quantify small molecules for research and development, or simple, fast, and repeatable QA/QC. Improve throughput by attaching the X-Auto autosampler

- Batteries – total analysis of liquid electrolyte including chemical and physical properties, quantification of mass transport and conductivity for electrolyte development, even below room temperature

- Industrial QA/QC – reliable quantification and identification of reactants, intermediates and products

- Chemical Research – the flexibility of X-Pulse 90 makes it ideal for the multi-user labs and core instrument facilities

- Chemical Manufacturing – robust QA/QC for rapid identification of samples, easily inserted into existing analysis workflows to complement existing techniques

- Polymers – determine average molecular weight or analyse synthesis in flow with ease

- Teaching NMR – teach fundamentals and engage students by using examples containing more exotic nuclei
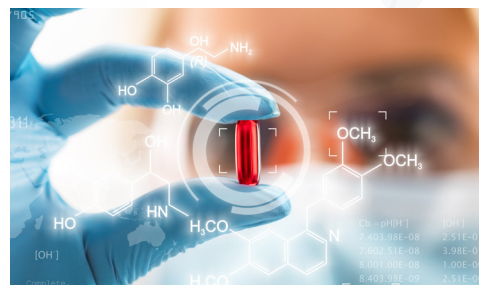
# X-Pulse 90 Accessories: Customise your Benchtop NMR Spectrometer

Several accessories can be added to the X-Pulse 90 to increase throughput, enable automation and remote operation, and to perform experiments/conduct analyses under certain, controlled conditions (e.g., different temperatures, in a flow regime).

As X-Pulse 90 continues the X-Pulse ethos of modularity and upgradeability, you can upgrade your X-Pulse 90 with all these accessories at any time.

Flow Cell

X-Pulse 90 equipped with a flow cell makes real time reaction control and mechanistic studies straightforward. The flow cell itself is simple to install owing to X-Pulse 90's removable probe. In addition, X-Pulse 90 features an external deuterium lock meaning reactions can be run and monitored without the need for expensive deuterated solvents. The orientation of the X-Pulse 90 diffusion gradient will ensure accurate measurement, even whilst the sample is flowing, and the excellent stability of X-Pulse 90 ensures the only variation you will see in the spectrum comes from the reaction itself.
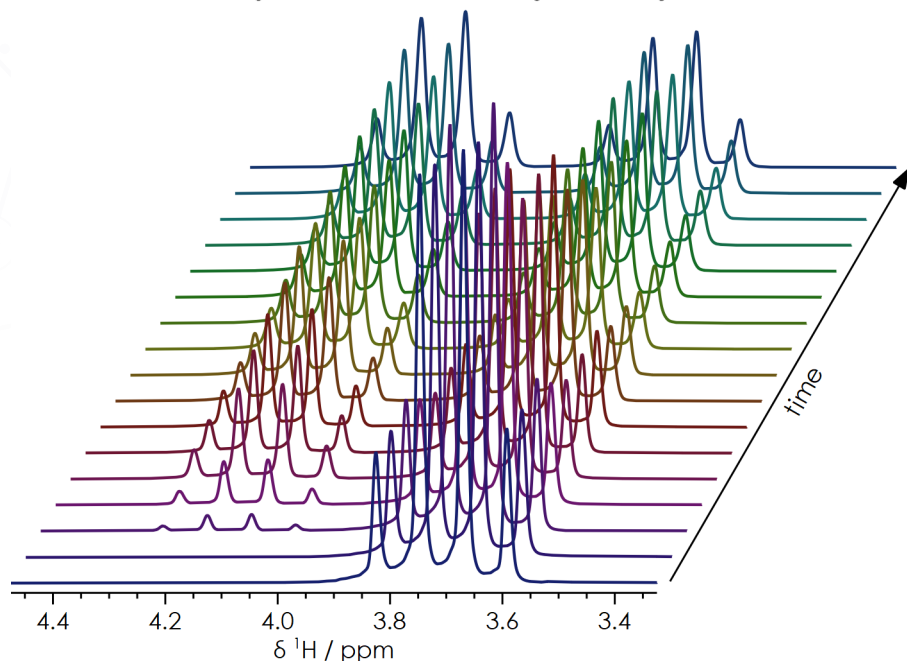
[1]H spectra of the reaction of ethanol and acetic acid, monitored by flowNMR. As the reaction progresses, ethanol is consumed (quartet at 3.7 ppm) and ethyl acetate formed (quartet at 4.1 ppm).

Variable Temperature (VT)

It is possible to combine the high sensitivity, X-Pulse 90 with the widest variable temperature (VT) range (0-60˚C) available for a benchtop NMR spectrometer. This allows a comprehensive understanding of reaction kinetics, as well as enabling users to observe a wider range of reactions. The large temperature range also facilitates investigation of the behaviour of mixtures at different temperatures, for example, quantifying battery electrolyte performance over a range of temperatures, including below room temperature.
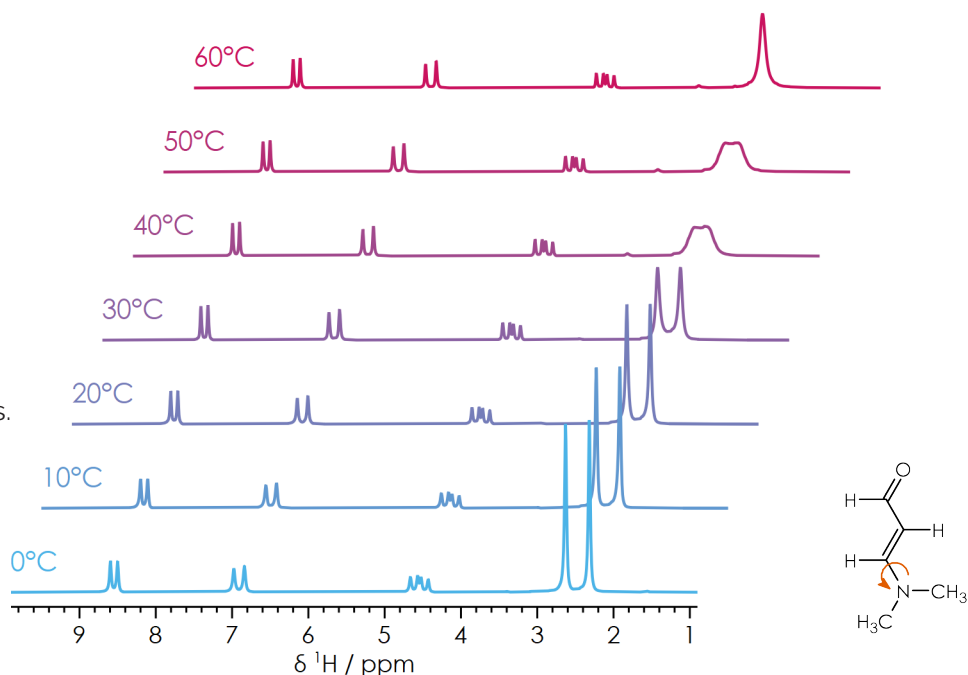
[1]H spectra of 3-dimethylaminoacrolein at 0 to 60˚C. As the temperature increases the two methyl signals coalesce into a single peak.

Automation with X-Auto

X-Pulse 90 equipped with an X-Auto autosampler can supercharge throughput and deliver a step change in productivity in busy environments and where instrument time needs to be maximized. The 25 position autosampler enables automated data collection and improves return on investment by allowing remote and time effective running of the spectrometer. The autosampler is installed with minimum instrument downtime and is fully controlled through the software enabling experimental queues to be created and saved with ease.

X-Pulse 90 Hardware Specifications

Magnetic field strength (operating frequency)	90 MHz
Sensitivity	>320:1 for ^{1}H on a ^{1}H/^{19}F only system (^{1}H 1% ethyl benzene) >240:1 for a dual channel probe (^{1}H 1% ethyl benzene)
Resolution	20% $CHCl_3$ in acetone-d$_6$: Linewidth at 50% <0.35 Hz Linewidth at 0.55% <15 Hz
Nuclei Available	As standard: ^{1}H and ^{19}F Dual-X: Choose two nuclei from our broadband range Broadband: All nuclei resonances ^{29}Si - ^{31}P (19%-41% ^{1}H)
3D Pulse Field Gradients	x, y, z >0.5 T/m diffusion gradient (z) as standard
Autosampler Compatible	X-Auto* - 25 positions
Variable Temperature Range	0-60˚C*
Size	Magnet 39 cm × 54 cm × 43 cm Electronics 37 cm × 52 cm × 26 cm
Weight	Magnet: 115 kg Electronics: 22 kg
NMR Tube Compatibility	4 mm and 5 mm diameter 7 inch minimum
PC	Windows PC and Monitor Included as Standard

*Options

X-Pulse 90 Software

Our acquisition software, SpinFlow, is easy-to-use and suitable for all levels of operators from experts to infrequent users.

- Walk up and collect 1D and 2D NMR data with one click and pre-set experiments
- Set your own parameters and save experiments
- Create and save experiment queues for consistent data acquisition
- Write and execute your own pulse sequences with full control of the whole spectrometer in a Python® - based language

Visit **nmr.oxinst.com/x-pulse-90**

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