



Спектрометр Aspect AI-60

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1H NMR Reaction Monitoring at 60 MHz

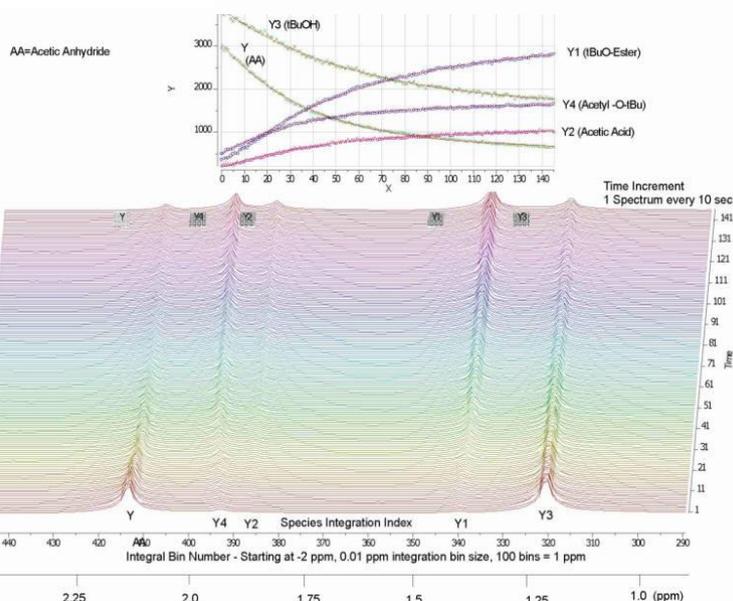
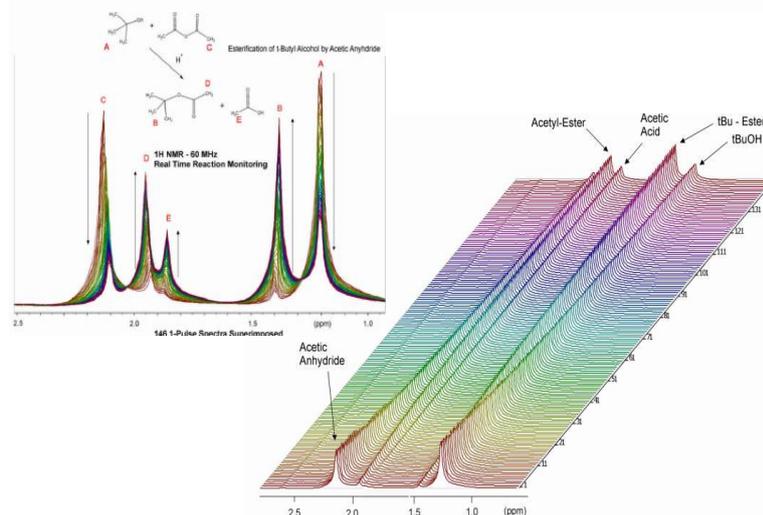
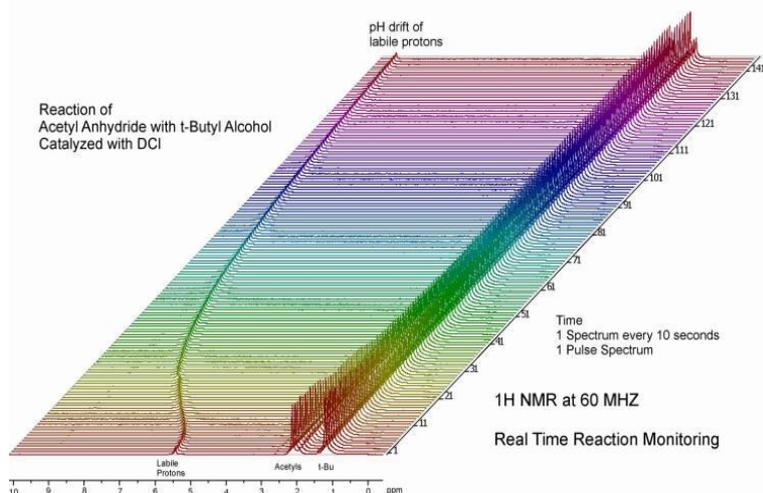
The use of an NMR as a simple flow detector for bench top reaction monitoring, mixing monitoring, dilution monitoring, or conversion monitoring has been limited by the need to bring the "reaction" to the typical "supercon" NMR lab. With the Aspect AI-60 system continuous flow NMR can be now be performed "at the bench." The system uses a high resolution 60 MHz permanent magnet with a simple flow cell and total system volumes of 2 to 5 ml depending on the length and diameter of the transfer tubing. Further, detection limits of analytes in the 200+ ppm range are possible without the use of typical deuterated NMR solvents. Analysis times of 5 to 20 seconds are achieved at flow rates of 1 to 20+ ml/minute.

Here are examples of the data visualization and rapid reaction profiling at 60 MHz the reaction for the esterification of tert-butanol with acetic anhydride in the presence of acid obtained every 10 seconds (1 pulse) over the course of 25 minutes.

The full width spectral plots in the upper right figure show the entire 25 minute reaction. As can be seen, the time dependent spectral changes are followed as the conversion reaction proceeds. In these spectra, the pH dependent change in the hydroxyl (OH) protons are readily observed.

In the figure to the immediate right the expansion plots corresponding to the CH₃ region of the 1H NMR spectrum are shown. Peak assignments corresponding to the constituents of the reaction are given. Excellent resolution of each CH₃ resonance from each constituent in the reaction (t-butyl alcohol, acetic anhydride, t-butyl methyl ester, and, acetic acid) are well resolved.

Integration of each peak allows quantitative determination of each constituent's concentration over the course of the entire reaction. As shown in the lower right figure, reaction kinetics can be determined. The Aspect AI-60 system's small footprint, high sensitivity, excellent resolution, and automated processing routines enable new opportunities and applications for reaction monitoring by NMR.



Aspect AI-60 60 MHz High Resolution FT-NMR System for Laboratory and At-Line Applications



Advantages

The Aspect AI-60's permanent magnet design requires no cryogenics as the system is powered by one standard wall outlet (110/220v). Samples can be run neat, in conventional protonated solvents, or, in deuterated NMR solvents. Deuterated solvents are not required. Probes accept standard 5 mm or 10 mm NMR tubes. Flow cell options are also available. Software operates under Windows® 7 or Windows® XP. Complete automation of all NMR tasks (Acquisition, Processing, Integration, Results Reporting) enable walk-up applications with minimum user training and/or experience. Spectral processing facilitates use of a variety of chemometric based routines for multiple property measurements.

Specifications

Field Strength at 45°C	1.4 Tesla
Fringe Field	Less than 1 gauss Clear Bore Size 30 mm diameter
Operating Frequency	60.1 ± 1MHz ¹ H 54.6 ± 1MHz ¹⁹ F 24.3 ± 1MHz ³¹ P
Dimensions (HxWxD)	37.5 x 22 x 24 inches 560 x 460 x 460 mm
Weight	~325 lbs ~160 Kg
Lab Probes	5 mm, 10 mm, and, Flow Through
Non-Spin Resolution	Less than 4 Hz at half height and less than 20 Hz at 1/10 height
Line Shape (5 mm)	Less than 80 Hz at the average peak height of ¹³ C satellites (0.55%)
¹ H Sensitivity	>25:1 (S/N), 1 pulse, 1% ethyl- benzene (CH ₃) in CDCl ₃
¹ H Pulse	<20 µsec 90° flip angle at 7 watt RF power for 5mm probe (Q of 150)

По вопросам продажи и поддержки обращайтесь:

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