# AT-PMSC-I

LOW-TEMPERATURE WIDELINE AUTOTUNING AND GONIOMETER NMR PROBE SYSTEM

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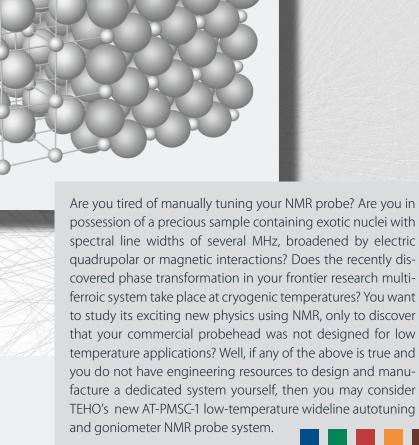
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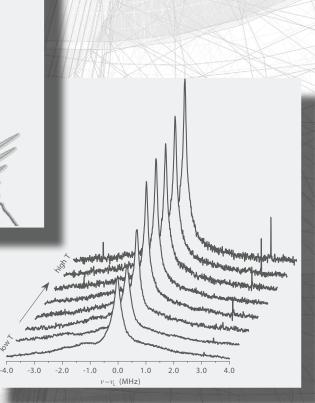












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# ATC-400 Digital Autotuning Controls

#### Automated wideline NMR

AT-PMSC-1 is an automatic tuning and matching system for NMR spectroscopy, consisting of a wideline research-grade goniometer probe, detachable stepper motor drive unit, high/low power RF switch, and CompactPCI-based controller unit with touchscreen interface. It provides for automatic tuning of RF resonant circuits in NMR experiments with X-nuclei resonance frequencies up to 400 MHz. Its application areas span from wideline NMR of disordered solids where spectra are acquired using point-by-point frequency scan (frequency-stepping) methods, to investigations of smeared phase transitions via NMR of low-sensitivity nuclei or low-concentration samples where detuning takes place due to temperature-dependent capacitance and inductance of the trimming elements of the NMR detection circuit.



### Easy integration

AT-PMSC-1 is typically integrated into the RF detection circuit of the spectrometer by an in-line connection of the remotely controlled RF switch, immediately in front of the probe. The RF switch is used to redirect the RF line of the NMR probe from the autotuning controller to the NMR spectrometer during the signal acquisition mode. In this way, operation of AT-PMSC-1 that is independent of spectrometer's hardware is achieved; no RF or I/O connectivity between the spectrometer and AT-PMSC-1 is required.



### Remote control

If the autotune functionality is needed in the course of experiment, it can be controlled via the RS-232/Ethernet connection from the workstation which controls the operation of the spectrometer. Specifically, the synchronization of automatic tuning of AT-PMSC-1 with the spectrometer is established through AT-PMSC-1 procedure calls from within the spectrometer automation sequences (e.g. Python or C-based automation programming). This functionality is provided with all modern spectrometers.



#### Modular design

AT-PMSC-1 is an automatic tuning and matching system for NMR spectroscopy which consists of four components:

- ATP-CF wideline multipurpose probe, equipped with up to four trimmer capacitors (room-temperature range or cryogenic-temperature range versions) and high precision goniometer
- ATM-C4G rapidly detachable stepper motor unit for mounting onto ATP-CF, with trimmer status LED display panel

tors allow for a quick attachment or detachment of the ATM-C4G stepper motor unit. When the stepper motor unit is detached from the ATP-CF or not powered, the ATP-CF probe, specifically the trimmer and goniometer shafts, can be rotated manually for setup purpuses. The ATM-C4G stepper motor unit is designed with industry-standard high power hybrid stepper motors and differential encoders so that it can be controlled with conventional stepper motion controllers. Your expensive, high-Q, cryogenic trimmer capacitors are protected from mechanical damage by adjustable limit switches.

- ATS-500 RF switch with status LEDs
- ATC-400 digital controller unit with touchscreen display

The ATP-CF probe is designed to fit into the Oxford Instruments Spectrostat<sup>NMR</sup> wide-bore cryostats of  $\Phi = 2.5''$ (model ATP-63G-CF) or  $\Phi = 2''$  (model ATP-51G-CF) bore inner-diameter. The probe is built to last: the housing material is highly corrosion-resistant non-magnetic stainless steel, the probehead base plate is made of titanium and the goniometer is machined from Vespel, delivering an exceptional wear resistance and hassle-free performance even at cryogenic temperatures. Stainlessteel ball-bearings are used to seat the trimmer and goniometer vacuum-sealed shafts. The mating shaft adap-



## Custom applications

Special care has been taken to ensure customizability of the probe, e.g. use of solenoids of various sizes and shapes, easy replacement of trimmer capacitors, and installation of additional mechanical, electrical, and optical components that may be needed in a customdesigned experiment. This is achieved via vacuum sealable access holes in the probe housing with preinstalled vacuum-tight multipole connectors with internal pinning, providing for easy attachment of RF circuits and wiring of external sensors, fiber-optic elements, and power supplies. The installation of user-designed coils has been made easy through the use of a rapidexchange coil holders. The standard NMR detection circuit featuring an irradiation/detection coil and two trimming elements for tuning and matching can be upgraded to four trimming elements. Specifically, a second pair of variable capacitors can be installed, allowing for even broader frequency tuning range in the frequencystepping experiments (typically beyond 20 MHz) or for double resonance experiments. The use of solder has been reduced to a minimun when assembling the probe parts. Nevertheless, care has been taken to retain the required level of electromagnetic shielding performance. All mechanical parts can be disassembled using only a screwdriver. For a researcher with engineering skills, this makes it simple to alter the existing parts or to add custom-designed probe parts in order to expand the functionality of the probe.

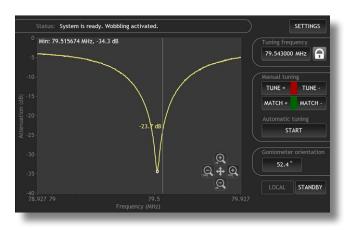


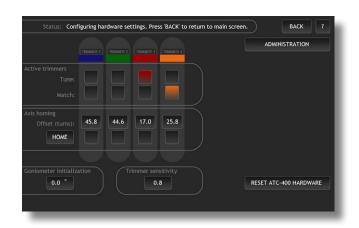
per motor unit is powered directly from the ATC-400 via a single cable harness. The controller also provides power, control, and RF tuning signal for the ATC-500 RF switch via two additional cables. Complete wiring of the AT-PMSC-1 autotuning system into an existing NMR spectrometer is thus achieved by solely three, ready to use, flexible cables. Moreover, cabling lengths can be as much as 20m or more since optically-coupled and differential-type signalling is employed. Distant positioning of the NMR magnet, across a large lab from the NMR spectrometer, therefore presents no obstacle for the installation of the AT-PMSC-1 autotuning system.

#### Versatile operation

The ATC-400 controller unit can be used as a standalone device, i.e. as a wobbler, to tune any RF resonant circuit. This is particularly useful in the preparation phase of an NMR experiment whenever user designed RF coils are used in order to improve the S/N ratio or to expand the frequency range of the probe tunability. The controller unit is based on the industrial-grade CompactPCI platform fitted with Intel Core 2 Duo CPU blade and digital RF synthesizer. A separate internal power supply provides power to integrated RF reflecometer and stepper motor controller and drive units. The ATM-C4G step-



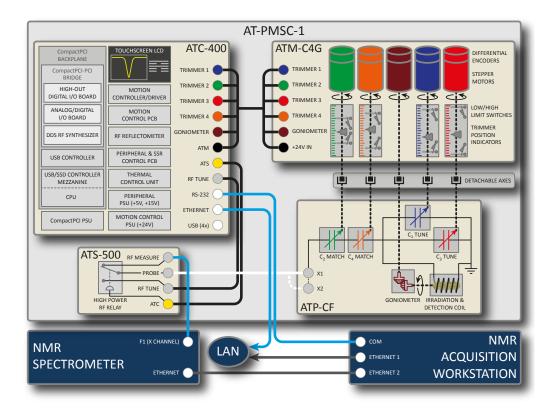




#### Touchscreen user interface

Through the ATC-400 touchscreen user interface, up to 4 trimmers and the goniometer of the ATP-CF probe can be controlled. The main screen of the interface displays a reflected RF power level vs. frequency and the orientation of the gonoimeter in real time, as well as the status bar. There are two modes of operation, the local one which, in addition to automatic tuning, allows for manual adjustment of trimmers and goniometer, and the remote one, intended for spectrometer-controlled autotuning and reorienting of samples. ATC-400 settings are controled through a separate screen, typically used to select active trimmers, to initialize the positions of trimmer and goniometer shafts, and to access the

online help. Although the application software runs on top of Microsoft Windows XP, the OS is hidden from the operator's access. The complete ATC-400 software layer can be automatically restored or upgraded by inserting a bootable USB key when the system is powered-on. Frequency-stepping experiments in a broad frequency range (several MHz) as well as temperature-dependence experiments in a broad temperature range (several hundred K), which require precise tuning at each step, are easily performed by issuing string-based commands to the RS-232 bus from the automation macro programs being executed on the NMR spectrometer.



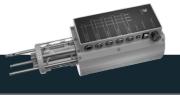
## Technical specifications



#### ATC-400 digital controller

General	
dimensions (W x D x H)	44.9 cm x 37.5 cm x 31 cm (17.7″ x 14.8″ x 12.2″)
without feet and handles	indistry-standard 19" 7U rack mountable, EMI shielded case
weight	25 kg (55 lbs)
housing material	chromated aluminium, surface paint in RAL 7038 color
power input rating	125/250 V AC, 50/60 Hz, 3 A
RF reflectometer	
frequency sweep generation	DDS
frequency range	10 - 400 MHz
accuracy	1 ppm
output impedance	50 Ω
reflectometer range	0 - 50 dB
Stepper motor control	
no. of channels	5 (4 x trimmer with limit switches, 1 x goniometer)
max. current	1.5 A/channel
inputs	2 x limit switch/channel, 1 x differential encoder/channel,
	motor status, emergency stop
Data acquisition and processing ha	rdware
platform	32-bit CompactPCI
CPU unit	Intel Core Duo 2.26 GHz
DAQ	PCI bus, 16-bit, 1MS/s sample rate
remote connectivity	RS-232, Ethernet
Operator panel (front)	
switches	on/off switch with two-color LED indicator
status indicators	standby mode LED
	remote mode LED
connectors	3 x USB 2.0
display panel	LCD, resistive touchscreen diplay size (diagonal): 12.1", 16:10
	resolution: 1280 x 800
Operator panel (back)	
switches	main power on/off switch
connectors	line power with fuse holder and line filter
	trimmers 1 - 4 : 19-pin female, color-coded
	goniometer: 19-pin male, color-coded
	ATS (to RF switch): 6-pin female
	ATM (to stepper motor unit): 4-pin female
	RF tune: type N female
	1 x USB 2.0
	1 x Ethernet
	1 x RS-232

Software	
background OS (hidden from the operator)	Microsoft Windows XP SP3
main screen	hardware status line reflected power level vs. frequency plot panel with zoom buttons and level indicators input/display fields for tuning frequency (with lock) and goniometer orientation manual tuning and automatic tuning buttons mode selection buttons
settings screen	active trimmers selection panel trimmer drive mechanism initialization buttons goniometer orientation initialization button help system access button OS and remote configuration buttons
remote control	via RS-232 or Ethernet, string-based command language



#### ATM-C4G stepper motor unit

General		
max. diameter	Φ 13 cm (Φ 5.1″)	
full height (including supports)	34 cm (13.4")	
weight	3.2 kg (7 lbs)	
materials	housing: chromated aluminum, surface paint in RAL 7038 color	
	supports: non-magnetic stainless steel	
	limit switch compartment cover: transparent acrylic glass	
power input rating (logic circuits)	+24 V, 500 mA DC	
Stepper motors		
number of axes	3 - 5 (2 - 4 with low/high limit sensors, goniometer axis without limit sensors)	
max. current	0.67 A per axis, powered from the autotuning controller	
holding torque	127 Nmm (18 oz-in)	
size and winding type	NEMA-11, bipolar serial	
overheat protection	microcontroller-based with fan	
Encoders		
resolution	500 steps/revolution	
zero-position signal	yes	
cable drivers	differential	
Limit switch compartment		
limit switch type	mechanical microswitch with adjustable position	
variable capacitor support	max. 100 turns full range	
position indication	sliding limit switch trigger	
	$\pm$ 50 turns, color-coded scales	
Operator panel		
switches	on/off switch with LED indicator	
	emergency switch	
status indicators	motor activity LEDs (5 x)	
	limit switch LEDs (8 x)	
connectors	trimmers 1 - 4 : 19-pin female, color-coded	
	goniometer: 19-pin male, color-coded power & status: 4-pin female	
	power a status. 4-pin remaie	

ATP-CF probe	
General	
compatibility	for use with Oxford Instruments Spectrostat <sup>NMR</sup> continuous flow CF-1200 cryostat
max. diameter	Φ 61.5 mm (Φ 2.42"), model ATP-63G-CF Φ 48.8 mm (Φ 1.92"), model ATP-51G-CF
full length (including shafts)	30 cm - 120 cm (11.8" to 47.2"), model ATP-63G-CF 30 cm - 60 cm (11.8" to 23.6"), model ATP-51G-CF exact dimensions are to be privided by the customer
weight	3.5 kg (7.7 lbs) at 90 cm (35.4") length, model ATP-63G-CF 2.5 kg (5.5 lbs) at 50 cm (19.7") length, model ATP-51G-CF
materials	housing: stainless steel, non-magnetic, high corrosion resistance goniometer: Vespel probehead base: titanium
temperature range	4K - 400 K, limited by the operating temperature range of trimmer capacitors
trimmer/goniometer adjustment	manual or stepper motor-controlled mechanical coupling to drive unit via male shaft couplers
vacuum sealing	rotary components (shafts): spring loaded bearing seals connectors: gasket seals
RF resonant circuit	
type	parallel, 2 - 4 trimmer capacitors
trimmers	<ul> <li>variable trimmer capacitors, standard or cryogenic version, extended shaft</li> <li>0.5 pF min. capacitance, 70 pF max. capacitance,</li> <li>various capacitance ranges and working voltages available</li> <li>20 - 105 turns full range</li> <li>max. shaft torque 70 Nmm (10 oz-in)</li> <li>76 mm (3") max. length, Φ 18 mm (Φ 0.7") max. diameter</li> </ul>
trimmer mounting	two grounded mounting holes for tuning capacitors two isolated (Teflon or Vespel) mounting holes for matching capacitors
trimmer rotational life	10,000 to 100,000 turns
irradiation/detection coil <sup>(*)</sup>	solenoid, saddle or other shapes rapid exchange coil holders (two pin male plug, Teflon base) for coil soldering Φ 20 mm (Φ 0.8") max. sample diameter 30 mm (1") max. sample length, model ATP-63G-CF 20 mm (0.8") max. sample length, model ATP-51G-CF
coil mounting	female socket, Teflon isolation, fixed into titanium probehead base
RF conductor	2 x semi-rigid, 50 $\Omega$ copper coaxial cables
external connectors	2 x N type female
internal connectors to trimmers	2 x SMA female, replaceable male counterpart with bare rigid cable termination
Goniometer	
gear ratio	36:1 (10°/revolution)
resolution	0.02°
positioning accuracy sample holder seating	$\pm$ 0.5° hexagonal, with fixing screw
max. sample holder dimensions	(*)see coil data above
Auxiliary inputs	
sensor connector S1	5-pin female
power connector S2	2-pin male, I <sub>max</sub> = 4 A, V <sub>max</sub> = 1 kV
spare hole	$\Phi$ 10 mm, vacuum-sealed when not used

#### ATS-500 high/low power RF switch



General	
dimensions (W x D x H)	10.5 cm x 10.5 cm x 5 cm (4.1" x 4.1" x 2")
weight	0.5 kg (1.1 lbs)
housing material	chromated aluminium, surface paint in RAL 7038 color
Electrical characteristics	
frequency range	DC – 2 GHz
max. CW power	400 W @ 500 MHz
max pulsed power	> 1.5 kW @ 500 MHz
impedance	50 Ω
actuator	electromechanical, failsafe, unused port terminated (5 W max.)
actuation signal	ΠL
max. stray magnetic field	10 G (1 mT)
Mechanical characteristics	
switching speed	< 20 ms
life	1.000.000 cylces
Operator panel	
status indicators	high/low power LEDs
connectors	probe: type N female
	RF measure: type N female
	RF tune: type N female
	ATC (to autotuning controller): 6-pin female

## Notes





KMZ Zalar Miran s.p. Predjamska cesta 12 1000 Ljubljana, SLOVENIA Jeklotehna TEHO d.o.o. Cesta na Brdo 85 1000 Ljubljana, SLOVENIA

Tel. +386 1 423 54 50 office | +386 31 689 308 mobile e-mail: nmr@teho.com | web: www.teho.com