SHIMADZU
Excellence in Science

S-GCMS-B31

Gas Chromatograph Mass Spectrometer

Hydrogen: A Guide for Setting Up Your System With a Helium Alternative

Hydrogen: The Optimal Helium Alternative

With growing helium shortages, switching to hydrogen is a popular alternative. This guide will include the recommended hardware changes and outline application compatibilities and best practices for a seamless change

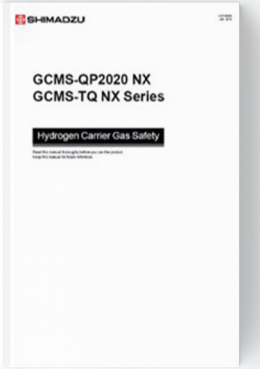
Precautions

Hydrogen gas may not be used for pressurizing headspace or thermal desorption equipment or used as a purge gas.

If you are using our HS-20 NX, TD-30, Purge and Trap, or have fitted an AOC-6000 Series with a purge gas for headspace, ITEX, or SPME conditioning, and are looking to move away from helium, please see our alternative options section of this document.

For a full list of cautions, please refer to the Hydrogen Carrier Gas Safety Guide. A copy is supplied with every instrument purchased and additional PDF copies can be obtained from your Sales Representative.

Additional documentation will be linked and referenced throughout this guide. Please contact your Sales or Tech Support Representative for more documents.

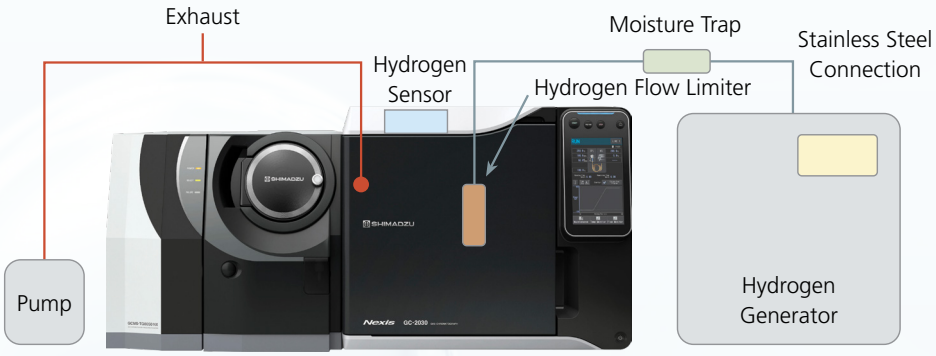


Find your local representative here!

01. HARDWARE

Overview

To adopt hydrogen as a carrier gas for GC-MS applications, a series of hardware add-ons are recommended to ensure safe usage. These range from gas connections, exhaust tubing, gas filter systems, gas flow controllers, hydrogen gas sources, and hydrogen gas sensors. Additionally, the selection of column and gas selector should be considered too.



A. Connections and Tubing

Hydrogen has been known to react with and degrade copper tubing. Over time, copper exposed to hydrogen becomes brittle and prone to leaks. Changing to stainless steel tubing is recommended. Connections specific to hydrogen are fitted with lefthand threads for added awareness and safety. Existing tubing may need to be retrofitted with different connectors to accommodate regulators.

Shimadzu LMF-MF stainless steel tubing 100 cm : 221-73555-00
Shimadzu LMF-MF stainless steel tubing 50 cm : 221-73555-50

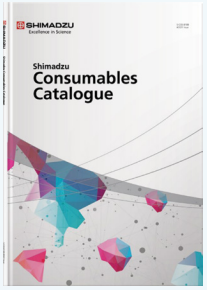
Adequate room ventilation is necessary; exhaust gas from the split vent should be discharged to a ventilation system to avoid the collection of hydrogen in the room. Care should be taken to ensure the gas does not stagnate in the ventilation system.

B. Filters

When using hydrogen from a hydrogen generator, water reduction is essential. Our moisture trap will help to reduce the amount of water introduced into the GC-MS system.

Hydrogen tanks may also have residual low-weight hydrocarbons. The Shimadzu triple filters are ideal for scrubbing these trace components for a clean background to your chromatography.

Filter	Part Number
Hydrogen Generator	
Big Moisture Kit	APASGT-C0BT1001S8
Hydrogen Tank	
Hydrogen Purification Filter Kit	APASGT-C01018S8
Triple Filter for Hydrogen	226-50752-10
Base Plate Single Position	226-50771-00



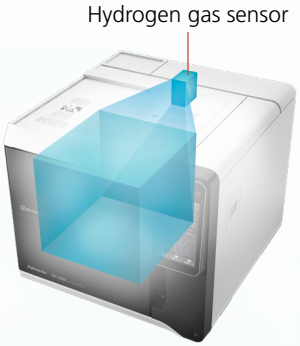
Check out our Shimadzu Consumable Catalogues to learn more about the gas filter kits.

C. Flow Limiter

To restrict excessive flow of hydrogen into the system in the unlikely event of electronic flow controller failure, flow limiters can be installed for the carrier gas flow line and detector flow line.

Shimadzu AFC hydrogen option : 221-87283-41
Shimadzu APC hydrogen option : 221-87280-41

D. Hydrogen Sensor



Part Number : 221-88999-41 (for Nexis and Brevis GC)

For added safety, a hydrogen leak sensor can be installed for the Nexis and Brevis GC oven in GCMS-QP2050, GCMS-QP2020 NX, GCMS-TQ8050 NX, and GCMS-TQ8050 NX systems. Linked to the gas line, upon detection of a leak, the sensor will provide a notification at 0.4% detection and immediately stop the flow of hydrogen carrier gas once hydrogen is detected at a 2% level. The sensor is configured to automatically shut down the instrument once a leak is detected and the flow shuts off.

E. Options: Tank or Generator for Supply of Hydrogen Gas

- Hydrogen Tank

A hydrogen tank is the fastest way to switch a lab over to using hydrogen carrier gas. When choosing a cylinder, ensure the purity is greater than 99.995% as outlined in the instrument site preparation documents.

While a tank is the lower maintenance option, contamination of the gas source must be taken into consideration. Hydrogen tanks are more likely to be contaminated with hydrocarbons; for that reason, careful monitoring of the filter system is recommended.

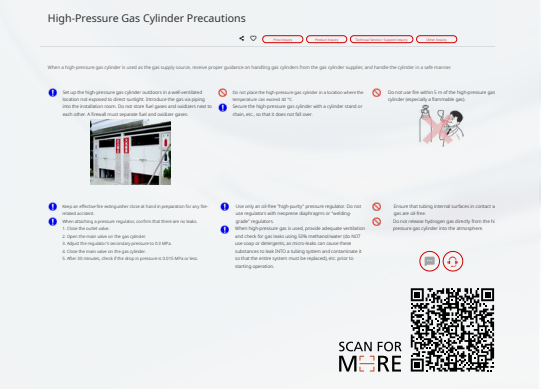
When using a tank, a regulator is needed to adjust for primary pressure into the GC; a two-stage regulator is most used and available directly from Shimadzu, with the following recommendations.

- Hydrogen Tank Regulator

Part Number : 221-35999-02

Hydrogen regulators are gas-specific with lefthand threads. Only use an oil-free high-purity pressure regulator as other regulators such as a welding grade type may lead to trace contamination with hydrocarbons or other machining agents.

When using hydrogen, set the regulator to the minimum required outgoing pressure to avoid excessive losses in the event of a leak. Leak check frequently with a solution of 50% methanol and ultrapure water to maintain a leak-free system. For further information, please see our gas cylinder handling page on our website link on the right.



- Hydrogen Generator

Part Number : 64-0250 PEAK Precision Hydrogen Trace 250 mL/min
Part Number : 64-0500 PEAK Precision Hydrogen Trace 500 mL/min
Part Number : 3301768 PEAK Precision Hydrogen Trace 1200 mL/min

A generator is the safest, most efficient way of converting a lab to hydrogen use with a GC-MS instrument. The generators listed above are both trace-level generators from PEAK Scientific. Trace here refers to the purity of hydrogen being produced; this level is required for use with scientific instrumentation.

We recommend generators with capacities of 250, 500, and 1200 mL from PEAK Scientific. This measurement determines the output of hydrogen, and therefore the number of instruments that can be simultaneously operated using the same generator. A 250 mL generator is recommended for laboratories with a single GC-MS. Adding more instruments to a low-output generator will lead to flow control issues and that may manifest as leak errors and is therefore not recommended. For laboratories with more instruments requiring hydrogen, the 500 or 1200 mL high-output generators can be plumbed to operate more instruments simultaneously.

The key benefits of a generator are safety and ease of use. Since generators produce hydrogen on demand, the total volume of hydrogen stored in the generator chamber is small – usually about 2L – which if completely vented into a regular lab space will not reach the 4% mixture level with the atmosphere. This significantly decreases the risk of using hydrogen, as there is no storage component risking large volume releases into the laboratory space to the point of flammability.

Furthermore, the generators can be coupled with a leak sensor that will shut down the generator in the event of a detected leak for added safety. As the generators take water as their hydrogen source, the added benefit to a generator is the easy replacement of just a water tank, instead of a high-pressure hydrogen cylinder.

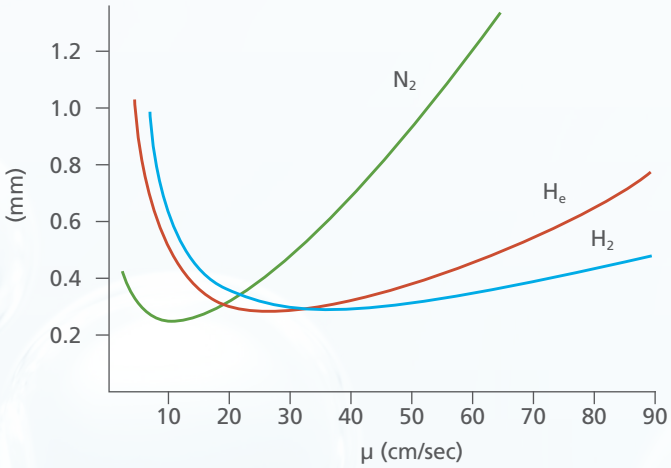
Due to water being the source of hydrogen, a high-capacity moisture filter is recommended to reduce moisture going into the instrument. This is different from tank hydrogen in that there is no risk of hydrocarbon contamination, removing the necessity for a triple filter.

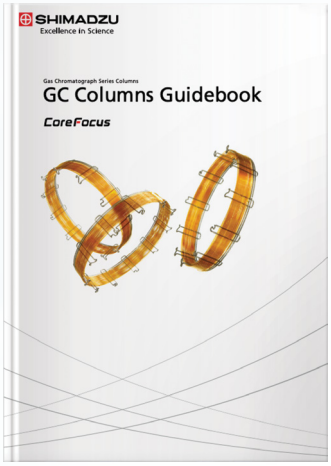
02. OTHER CONSIDERATIONS

Columns

Hydrogen, being a lighter gas, results in faster chromatography. For optimal separation, smaller inner diameter columns are recommended.

Shimadzu's constant linear velocity carrier gas control mode seamlessly controls the optimal pressures and flows to keep the linear velocity at its most optimal throughout a temperature program. Using constant linear velocity, you can be confident in consistent chromatography throughout your programming.



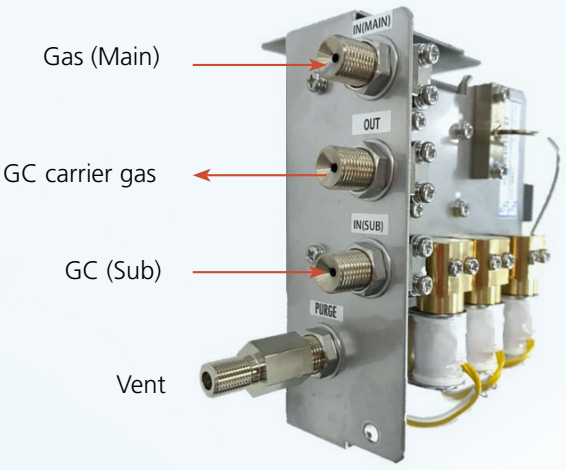


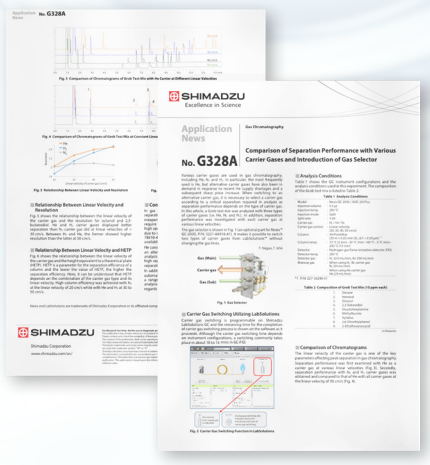
Unlike nitrogen, hydrogen behaves more closely to helium in that as linear velocity changes, the height equivalent of theoretical plates (HETP or H) will remain low over a larger range of velocities, resulting in optimal chromatography. This can be visualized by how closely the Van Deemter plot of hydrogen follows that of helium.

- Gas Selector

Part Number : 221-84916-41

Needing to switch back and forth between carrier gases?
The gas selector is the solution to manual tubing removal and exchange.





Compatible with GCMSsolution version 4.53 (and later) and both LabSolutions GC and GCMS software, the most popular use of the gas selector is to use an alternative gas during instrument downtime to avoid carrier gas losses while idle. This functions similarly to our Eco mode as it can be configured to start after a batch; for example, to run for the remainder of the night until a user reset in the morning. Upon returning to regular carrier gas, it is recommended to wait 30 minutes to allow the system to stabilize and flush out the substitute gas.

Vial#	Sample Name	Method File	Data File	Level#	Run Mode	Analysis Type
1	Pesticide-1	SIM.qgm	pest_std_001	1	DL AQ DP	IT QT
2	Pesticide-2	SIM.qgm	pest_std_002	2	DL AQ DP	IT QT
3	Pesticide-3	SIM.qgm	pest_std_003	3	DL AQ DP	IT QT
4	Pesticide-4	SIM.qgm	pest_std_004	4	DL AQ DP	IT QT
0	Blank	Switch to Subgas.qgm	blank_001	1	DL AQ DP	IT QT

Another option with the gas selector is to change carrier gas for specific applications where one gas is desired over the other.

Two gas selectors are configurable on a single GC-MS if two analytical lines are desired. This configuration is recommended over a selector on a T-connection, as additional dead volume of the line will require longer flush times. The separate gas selectors can be configured with different substitute gases.

The gas selector is designed for the Nexis and Brevis GC used on the GCMS-QP2050, GCMS-QP2020 NX as well as GCMS-TQ8040 NX and GCMS-TQ8050 NX. Contact your local Shimadzu representative for a recommendation of gas selector for GC-MS systems with GC-2010 series.

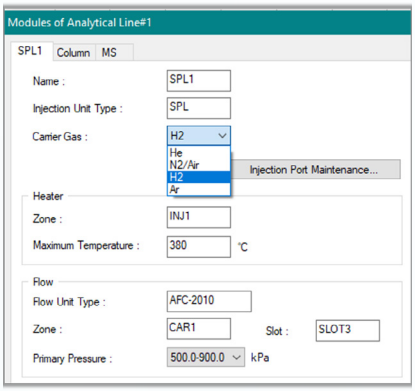
03. SOFTWARE

System Configuration

Carrier gas can be set from the system configuration for each analytical line. This option is best for one-time transitions to constant hydrogen use, where a gas selector is unnecessary.

Selecting the SPL in the analytical line to be converted will bring up the modules available. The carrier gas options can be found in a drop-down in the modules window.

Since the setting is dependent on the analytical line, this enables a system configuration with different carrier gases for a 2-inlet and 2-detector system.



Method Conversion

EZGC METHOD TRANSLATOR

For easy method conversion, we recommend Restek's EZGC converter. This calculator tool allows the user to select different carrier gases, input the column parameters, and select the flow control mode. Click the image for a shortcut to the online calculator! For more detailed information on method conversion, please see our method development video on our YouTube channel.

SCAN FOR MORE

AART, Shimadzu's automatic adjustment of retention times software feature will allow for method conversion for both an acquisition and processing window adjustment.

Note that our Smart Databases already include the use of AART and have acquisition methods pre-built for use with the databases. Using the pre-built methods will provide optimal retention time when using either helium or hydrogen carrier gas.

Alternate Gas – Instrument Compatibility Table

Instrument	H_2 Compatibility	N_2 Compatibility
QP Series		
GCMS-QP2010	✖	✖
GCMS-QP2010 S	✖	✖
GCMS-QP2010 SE	✓[a]	✖
GCMS-QP2010 Ultra	✓	✓
GCMS-QP2010 Plus	✓	✓
GCMS-QP2020	✓	✓

Instrument	H_2 Compatibility	N_2 Compatibility
GCMS-QP2020 NX	✓	✓
GCMS-QP2050 (65 mL/min)	✗	✗
GCMS-QP2050 (265 mL/min)	✓	✓
TQ Series		
GCMS-TQ8030	✓	✗
GCMS-TQ8040	✓	✓[b]
GCMS-TQ8040 NX	✓	✓[b]
GCMS-TQ8050	✓	✓[b]
GCMS-TQ8050 NX	✓	✓[b]

[a] H_2 is not recommended for GCMS-QP2010 SE due to sensitivity losses, but it may be used in some cases
[b] N_2 is not recommended as a carrier gas for the TQ series due to the possibility of losses in both sensitivity and the optimization of MRM transitions but may be used for some applications

Instrument	H_2 Compatibility		N_2 Compatibility	
Sample Introduction	Purge Gas	Carrier Gas	Purge Gas	Carrier Gas
HS-20 NX	✗	✓	✓	✓
TD-30	✗	✓	✓	✓
AOC-6000 Series	✗	✓	✓	✓
Purge and Trap	✗	✓	✓	✓
Pyrolyzer	✗	✗	✓	✓

Sensitivity losses have been reported for some applications when converting to hydrogen carrier gas. This is primarily due to an increase in flow entering the MS due to the required higher flow rates for optimal chromatography. The increased flow of gas into the MS leads to a reduction in the mean free path of the ions from the source to the detector, leading to a drop in sensitivity. This is more pronounced in older instruments and the GCMS-QP2010 SE due to the lower volume capacity vacuum systems.

Alternative Options for Purging and Pressurizing Hydrogen gas

Hydrogen gas cannot be used for pressurizing headspace or thermal desorption sampling techniques, nor can it be used as a purge gas with the AOC-6000 Series or Purge and Trap systems.

As an alternative, nitrogen gas is proposed for use with these sampling techniques, either as the carrier gas or in tandem with hydrogen as the carrier.

AOC-6000 Series

The AOC-6000 series autosampler has a wide range of applications and sampling techniques, many of which use purge gas. Headspace and dynamic headspace via the HS and ITEX tools both use a purge gas within the tool itself. SPME using either the fiber or arrow configuration can include a conditioning station for inert thermal cleaning of the coating. For these applications, the alternatives to helium are nitrogen or argon gas.

The purpose of the purge gas in each of these cases is to ensure an inert environment for any sorbtive phases in the tools and to clear out any remainder of previous sample material to reduce carryover. As the gas is not used for separation, using nitrogen in these cases will not affect the chromatography, but will ensure your tools and materials are clean and ready to use.

HS-20 NX

The headspace sampler pressurizes each vial to ensure optimal sample introduction into the loop or trap. Due to the requirement to collect gas in the headspace oven, hydrogen gas cannot be used for the sample introduction technique. Instead, we propose a combination approach using nitrogen. Nitrogen can be used to purge the needle, pressurize the vial, and load the sample, all while using hydrogen as the carrier gas.

TD-30

The thermal desorber also requires the collection of gas during leak checks and system re-pressurization, which poses a significant risk when using hydrogen. Similar to the HS-20 NX, we propose a combination approach using nitrogen. Nitrogen can be used for pressurization while hydrogen is used as the carrier gas.

Purge and Trap

Similarly to the HS-20, the GL Sciences PT7000 purge and trap system allows for a dual gas setup. Due to the need to pass the extracting gas through the sample and force collection onto a trap, hydrogen is not recommended for the concentrator, however it can be used as a carrier gas. For further information and resources to optimize this change, please contact your local sales representatives for recommended specifications. Note that many applications using purge and trap are regulated. Please ensure the chosen carrier gas and purge gas meet the method specifications of regulations, if applicable.

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