Agilent
7200 Accurate-Mass
Quadrupole
Time-of-Flight GC/MS
System

Concepts Guide

The Big Picture

Agilent Technologies

Notices

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Software Revision

This guide applies to the Agilent MassHunter Workstation Software -- Data Acquisition for 7200 Quadrupole Time-of-Flight program version B.03.00 or higher until superseded.

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In This Guide...

The Concepts Guide presents “The Big Picture” behind the operation of the Agilent 7200 Accurate-Mass Quadrupole Time-of-Flight GC/MS System by helping you understand how the hardware and software work.

1 Overview

Learn how the 7200 Q-TOF GC/MS helps you do your job.

2 Theory and Inner Workings

Learn the concepts you need to understand how the 7200 Q-TOF works.

3 Agilent 7200 Accurate-Mass Q-TOF and Performance

Learn how the 7200 Q-TOF exceeds performance measures.

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1
Overview

This chapter provides an overview of the Agilent 7200 Accurate-Mass Quadrupole Time-of-Flight (Q-TOF) GC/MS system, its applications, and its data analysis system.

System Description

The Agilent 7200 Accurate-Mass Quadrupole Time-of-Flight (Q-TOF) GC/MS is a stand-alone quadrupole time-of-flight mass spectrometer for use with the Agilent 7890 Gas Chromatograph. The 7200 Q-TOF features:

- Three turbomolecular vacuum pumps
- Rotary vane foreline pump
- Independently MS-heated removable EI or CI ion source
- Removable ion source (RIS), which allows quick change from EI to CI source with minimal loss of vacuum in the instrument
- Independently MS-heated hyperbolic quadrupole mass filter, which can be heated to high temperatures, minimizing the contamination typical with low temperature analyses
- Single hexapole collision cell
- Vacuum-insulated flight tube with dual-stage ion mirror
- Fast electronics, allowing fast sampling rates
- Analog-to-digital detector
- Independently GC-heated GC/MS interface with automatic retraction during source removal

The 7200 Q-TOF incorporates a hexapole collision cell blanketed with nitrogen gas, to improve the ion fragmentation prior to detection quantification. It also includes new ion optics for focusing the ions prior to the flight tube and detector.

This configuration has advantages for many applications. The data is interpreted through the use of the MassHunter WorkStation software, which provides quantitative and qualitative analyses of the data obtained.

The 7200 Q-TOF can operate in either TOF mode or MS/MS mode. When operating in TOF mode, the instrument can obtain high resolution, accurate mass measurements, and fast full spectrum acquisition. MS/MS mode provides high resolution, accurate mass measurements, and fast full product ion spectra with high sensitivity. These features make the 7200 Q-TOF a good tool for solving complex analytical problems, resolving structural elucidation of unknowns, and confirmation of nontarget compounds.

Q-TOF applications

The 7200 Q-TOF GC/MS combination can quantify trace organic compounds in complex matrices. The following applications use this type of quantification:

- Food safety and research
- Environmental contaminants studies
- Toxicology
- Forensics
- Metabolomics and metabonomics
- Natural product research
- Human and animal doping studies
- Energy research and petrochemicals
- Homeland security

Paired with the Agilent 7890 GC, the 7200 Q-TOF delivers sensitive, reproducible analyses of target compounds in complex matrices. This provides the following:

- Femtogram-level limits of detection and quantification
- Selective quantification of target compounds in high chemical background samples
- Improved signal-to-noise ratios in complex matrices
- Ability to meet stricter regulations on sample analytical limits for certain applications
- Simplified operation with Agilent’s data analysis software
- Fast MS/MS operation
- Reproducible mass accuracy

The 7200 Q-TOF offers the improved sensitivity in GC/MS analysis that is required by many commercial and regulatory applications.

Instrument control software

The MassHunter WorkStation Instrument Control software allows you to perform the following tasks from a single window:

Prepare the instrument

- Start and stop the instrument from the software
- Download settings to the GC and the Q-TOF in real time to control the instrument
- Evaluate if the MS parameters are within the limits to produce the specified mass accuracy and resolution with a Checktune report
- Optimize MS parameters automatically (Autotune) or manually through Agilent tuning programs and print a tune report
- Monitor the actual conditions of the instrument
- View the real-time plot for chromatograms and instrument parameters (both GC and MS) and print a real-time plot report
- View the centroided line spectrum of a peak or the mass range profile spectrum of a peak in real time

Set up acquisition methods

- Enter and save the acquisition method parameter values for the GC and the Q-TOF
- Select and label the total ion chromatograms (TIC) or extracted ion chromatograms (EIC) that you want to appear in the real-time plot
- Set up time segments for each scan type and analysis where parameters change with the time segment or with the scans within the time segment
- Print an acquisition method report

Acquire data

- Enter sample information and pre- or post-programs (scripts) and run single samples interactively
- Enter and run both individual samples and automated multiple samples organized in a sequence
- Set up pre- and post-scripts to run between samples in a sequence
- Set up and run a sequence to optimize MS acquisition parameters
- Print a sequence report
- View system events, including start and stop times, run events and errors and print an event log report

To learn how to get started with the Agilent 7200 Q-TOF GC/MS, see the *Quick Start Guide* (G6845-90014).

To learn more about how to use the Agilent 7200 Q-TOF GC/MS with real samples and data, see the *Agilent 7200 QTOF Acquisition Familiarization Guide* (G6845-90011).

To learn how to do individual tasks with the GC/MS, see the *Online Help*.

To learn more about an Agilent 7890 GC, see the *Agilent 7890A GC Documentation.*

Data analysis software

Quantitative analysis program

Agilent has designed the MassHunter Quantitative Analysis program to help quantify very low amounts of material with the following unique features:

- Imports information directly from the acquisition method
- Provides a curve-fit assistant to test all fits and statistics on the calibration curve quality
- Integrates signals with an automated, parameter-free integrator that uses a novel algorithm, optimized for Q-TOF data

- Presents a batch results window to help you review and operate on an entire batch of data at once
- Automatically detects outliers
- Provides preconfigured templates for basic reporting and enables the capability to create custom reports in Microsoft Excel

Please refer to the *Agilent MassHunter Workstation Software - Quantitative Analysis Familiarization Guide* (G6845-90016) or the online Help for the Quantitative Analysis program.

Qualitative analysis program

For fast method development, this software is used to quickly review the qualitative aspects of the data, such as the optimum precursor to product ion transitions.

Agilent designed the MassHunter Qualitative Analysis program to present large amounts of data for review in one central location. With the program you can do these operations for any type of mass spectrometer data that you open:

- Extract chromatograms
- View and extract peak spectra
- Subtract background
- Integrate the chromatogram
- Find compounds

You can also set up methods to automatically do the tasks in the list, as well as others, when you open the data files.

Please refer to the Online Help for the Qualitative Analysis program.

2

Theory and Inner Workings

This chapter explains the inner workings of the 7200 Q-TOF GC/MS.

How Do Q-TOF Mass Spectrometers Work?

The Agilent 7200 Q-TOF is an orthogonal time-of-flight mass spectrometer. It performs MS/MS using a quadrupole and a hexapole, or collision cell, prior to a flight tube and detector. The sample is first ionized with either an electron impact (EI) ion source, or a chemical ionization (CI) ion source. After ionization, the ions pass through the quadrupole analyzer, which consists of four parallel hyperbolic rods through which selected ions are filtered, based on their mass to charge ratio (m/z).

The ions passing through the quad are then directed to the collision cell, which is set to select and fragment precursor ions into product ions. The collision cell is a hexapole filled with nitrogen, and is designed for axial acceleration, which helps with high speed MS/MS analysis. The fragmented ions, or product ions are sent through a slicer, which helps to focus the ion stream before they are sent through a flight tube to the detector.

The acceleration pulse applied to send the ions up the flight tube is orthogonal to the direction that the ions are leaving the mass analyzer. This geometry minimizes the effect of the entrance velocity on the flight time, leading to higher resolution. Once the ions reach the end of the flight tube, they bounce off a reflector, or dual-stage ion mirror and travel in a reverse path back down to the bottom of the tube. The analog-to-digital detector is located at the bottom of the flight tube. It counts the ions and sends a signal to the MassHunter software for data collection and analysis.

Sample Ionization Technology

In GC/MS, before the sample can be analyzed, it must be ionized in the ion source. There are two methods of ionization in GC/MS: electron impact (EI) ionization, and chemical ionization (CI).

Electrion Impact Ionization

In electron impact ionization mode, the sample stream enters an EI ion source from the GC/MS interface. Electrons emitted from a filament enter the ionization chamber, guided by a magnetic field. The high-energy electrons interact with the sample molecules, ionizing and fragmenting them. The positive voltage on the repeller pushes the positive ions into the lens stack, where they pass through several electrostatic lenses. These lenses concentrate the ions into a tight beam, which is directed into the quadrupole mass filter.

Source Body

The ion source body is a cylinder. It holds the other parts of the ion source, including the lens stack. With the repeller and the drawout plate, it forms the ionization chamber. The ionization chamber is the space where the ions are formed. Slots in the source body help the vacuum system pump away carrier gas and unionized molecules.

Filaments

Two filaments are located on opposite sides of the EI ion source body. The *active* filament carries an adjustable AC emission current. The emission current heats the filament causing it to emit electrons, which ionize the sample molecules. In addition, *both* filaments have an adjustable DC bias voltage. The bias voltage determines the energy on the electrons, usually –70 eV. The filament shuts off automatically if there is a general instrument shutdown. Three parameters affect the filaments: filament selection, filament emission current, and electron energy.

Filament selection

The filament selection parameter selects the filament in the ion source that is active. Since filaments may have some variability, we advise running a tune whenver a different filament is selected.

Emission current

The filament emission current (Emission) is variable between 0 and –315 µA, but should be set to the software default for normal operation.

Electron energy

The electron energy (EIEnrgy) is the amount of energy on the ionizing electrons. It is determined by the bias voltage; –70 VDC bias on the filament causes emitted electrons to possess –70 eV (electron volts). This value is adjustable from –5 to –241 VDC, but for normal operation, set this parameter to 70.

Magnet

The field created by the magnet directs the electrons emitted by the filament into and across the ionization chamber. The magnet assembly is a permanent magnet with a charge of 350 gauss in the center of the field.

Repeller

The repeller forms one wall of the ionization chamber. A positive charge on the repeller pushes positively charged ions out of the source through a series of lenses. The repeller voltage is also known as the ion energy, although the ions only receive about 20% of the repeller energy. The repeller voltage can be varied from 0 to +42.8 VDC. Some tune programs use a fixed repeller voltage. Others ramp the repeller voltage to find the optimum setting. Setting repeller voltage too low results in poor sensitivity and poor high mass response. Setting repeller voltage too high results in precursors (poor mass filtering) and poor low mass resolution.

Extractor lens assembly

The extractor lens assembly forms another wall of the ionization chamber. The ion beam passes through the hole in the extractor lens. The assembly is slotted. The slots correspond to slots in the source body. These slots allow carrier gas and unionized molecules to be pulled away by the vacuum system. The extractor lens assembly is at ground potential.

Ion focus

The voltage on the ion focus lens can be varied from 0 to –127 VDC. A typical voltage is between –70 and –90 VDC. In general: • Increasing the ion focus voltage improves sensitivity at lower masses. • Decreasing the ion focus voltage improves sensitivity at higher masses. • Incorrect ion focus adjustment results in poor high mass response.

Entrance lens

The entrance lens is at the end of the ion source, prior to the entrance of the quadrupole mass filter. This lens minimizes the fringing fields of the quadrupole, which discriminate against high-mass ions. There is a permanent +4.4 volt voltage added to the entrance lens. The total voltage applied to the entrance lens is the sum of the entrance lens offset and entrance lens gain and the +4.4 volt permanent offset. Entrance lens voltage = +4.4 VDC + offset + (gain × mass)

Chemical Ionization

Chemical ionization (CI) is a technique for creating ions used in mass spectrometric analyses. There are significant differences between CI and electron ionization (EI). This section describes the most common chemical ionization mechanisms.

In EI, relatively high-energy electrons (70 eV) collide with molecules of the sample to be analyzed. These collisions produce (primarily) positive ions. Upon ionization, the molecules of a given substance fragment in fairly predictable patterns. EI is a direct process; energy is transferred by collision from electrons to the sample molecules.

For CI, in addition to the sample and carrier gas, large amounts of reagent gas are introduced into the ionization chamber. Since there is so much more reagent gas than sample, most of the emitted electrons collide with reagent gas molecules, forming reagent ions. These reagent-gas ions react with each other in primary and secondary reaction processes that establish an equilibrium. They also react in various ways with sample molecules to form sample ions. CI ion formation involves much lower energy and is much more “gentle” than electron ionization. Since CI results in much less fragmentation, CI spectra usually show high abundance of the molecular ion. For this reason, CI is often used to determine the molecular weights of sample compounds.

Methane is the most common CI reagent gas. It yields certain characteristic ionization patterns. Other reagent gases yield different patterns and may result in better sensitivity for some samples. Common alternative reagent gases are isobutane and ammonia. Carbon dioxide is often used in negative CI. Less common reagent gases are carbon dioxide, hydrogen, Freon, trimethylsilane, nitric oxide, and methylamine. Different ionization reactions occur with each reagent gas.

Water contamination in reagent gases will decrease CI sensitivity dramatically. A large peak at m/z 19 (H_30^+) in positive CI is a diagnostic symptom of water contamination. In high enough concentrations, especially when combined with calibrant, water contamination will result in a heavily contaminated ion source. Water contamination is most common immediately after new reagent gas tubing or reagent gas cylinders are connected. This contamination will often decrease if the reagent gas is allowed to flow for a few hours, purging the system.

Positive CI Theory

Positive CI (PCI) occurs with the same analyzer voltage polarities as EI. For PCI, the reagent gas is ionized by collision with emitted electrons. The reagent gas ions react chemically with sample molecules (as proton donors) to form sample ions. PCI ion formation is more “gentle” than electron ionization, producing less fragmentation. This reaction usually yields high abundance of the molecular ion and is therefore often used for determining molecular weights of samples.

The most common reagent gas is methane. Methane PCI produces ions with almost any sample molecule. Other reagent gases, such as isobutane or ammonia, are more selective and cause even less fragmentation. Because of the high background from the reagent gas ions, PCI is not especially sensitive and detection limits are generally high.

There are four fundamental ionization processes that take place during positive chemical ionization at ion source pressures in the 0.8 to 2.0 Torr range. These are:

- Proton transfer
- Hydride abstraction
- Addition
- Charge exchange

Depending on the reagent gas used, one or more of these four processes can be used to explain the ionization products observed in the resulting mass spectra.

EI, methane PCI, and ammonia PCI spectra of methyl stearate are shown in Figure 1. The simple fragmentation pattern, large abundance of the $[MH]^+$ ion, and the presence of the two adduct ions are characteristic of positive chemical ionization using methane as a reagent gas.

The presence of air or water in the system, especially in the presence of PFDTD calibrant, quickly contaminates the ion source.

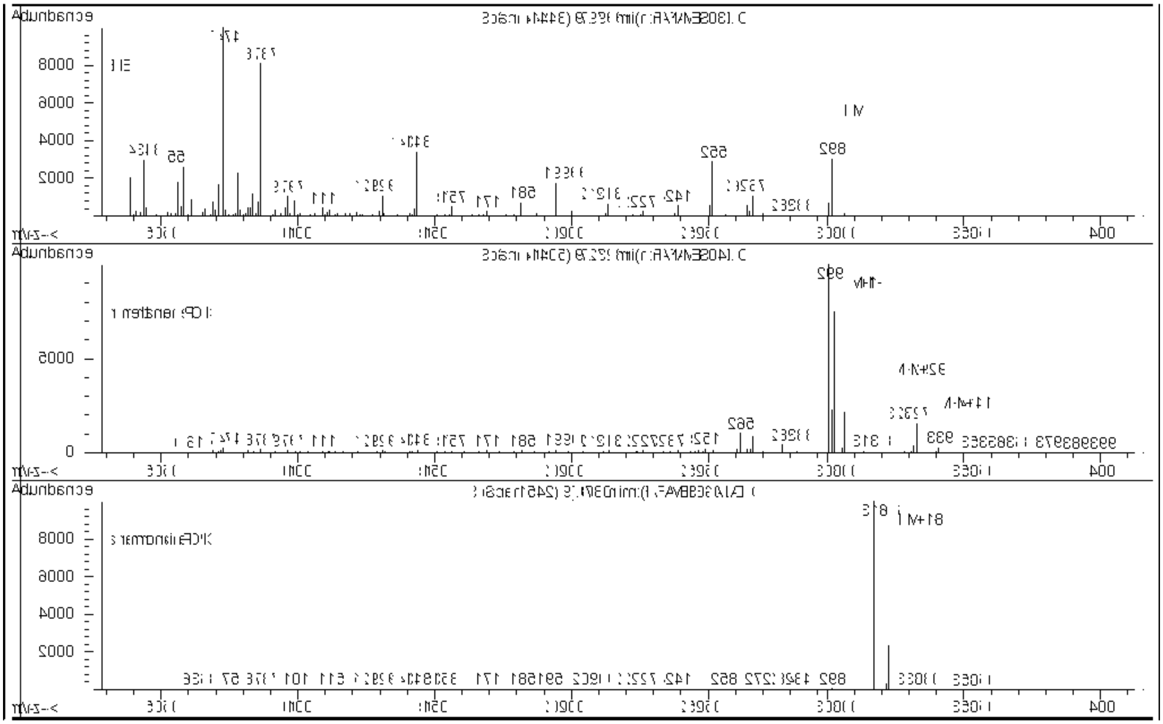


Figure 1 Methyl stearate (MW = 298): EI, methane PCI, and ammonia PCI

Proton transfer

Proton transfer can be expressed as

$$BH^+ + M \rightarrow MH^+ + B$$

where the reagent gas B has undergone ionization resulting in protonation. If the proton affinity of the analyte (sample) M is greater than that of the reagent gas, then the protonated reagent gas will transfer its proton to the analyte forming a positively charged analyte ion.

The most frequently used example is the proton transfer from CH_5^+ to the molecular analyte, which results in the protonated molecular ion MH^+.

The relative proton affinities of the reagent gas and the analyte govern the proton transfer reaction. If the analyte has a greater proton affinity than the reagent gas, then proton transfer can take place. Methane (CH_4) is the most common reagent gas because its proton affinity is very low.

Proton affinities can be defined according to the reaction:

$$B + H^+ \rightarrow BH^+$$

where the proton affinities are expressed in kcal/mole. Methane's proton affinity is 127 kcal/mole. Tables 1 and 2 list the proton affinities of several possible reagent gases and of several small organic compounds with various functional groups.

The mass spectrum generated by a proton-transfer reaction depends on several criteria. If the difference in proton affinities is large (as with methane), substantial excess energy may be present in the protonated molecular ion. This can result in subsequent fragmentation. For this reason, isobutane with a proton affinity of 195 kcal/mole may be preferred to methane for some analyses. Ammonia has a proton affinity of 207 kcal/mole, making it less likely to protonate most analytes. Proton-transfer chemical ionization is usually considered to be “soft” ionization, but the degree of the softness depends on the proton affinities of both the analyte and the reagent gas, as well as on other factors including ion source temperature.

Table 1 Reagent gas proton affinities

Species	Proton affinity kcal/mole	Reactant ion formed
H_2	100	H_3^+ (*m/z* 3)
CH_4	127	CH_5^+ (*m/z* 17)
C_2H_4	160	$C_2H_5^+$ (*m/z* 29)
H_2O	165	H_3O^+ (*m/z* 19)

Table 1 Reagent gas proton affinities (continued)

Species	Proton affinity kcal/mole	Reactant ion formed
H_2S	170	H_3S^+ (*m/z* 35)
CH_3OH	182	$CH_3OH_2^+$ (*m/z* 33)
t-C_4H_{10}	195	t-$C_4H_9^+$ (*m/z* 57)
NH_3	207	NH_4^+ (*m/z* 18)

Table 2 Proton affinities of selected organic compounds for PCI

Molecule	Proton affinity (kcal/mole)	Molecule	Proton affinity (kcal/mole)
Acetaldehyde	185	Methyl amine	211
Acetic acid	188	Methyl chloride	165
Acetone	202	Methyl cyanide	186
Benzene	178	Methyl sulfide	185
2-Butanol	197	Methyl cyclopropane	180
Cyclopropane	179	Nitroethane	185
Dimethyl ether	190	Nitromethane	180
Ethane	121	n-Propyl acetate	207
Ethyl formate	198	Propylene	179
Formic acid	175	Toluene	187
Hydrobromic acid	140	*trans*-2-Butene	180
Hydrochloric acid	141	Trifluoroacetic acid	167
Isopropyl alcohol	190	Xylene	187
Methanol	182		

Hydride abstraction

In the formation of reagent ions, various reactant ions can be formed that have high hydride-ion (H^-) affinities. If the hydride-ion affinity of a reactant ion is higher than the hydride-ion affinity of the ion formed by the analyte's loss of H^-, then the thermodynamics are favorable for this chemical ionization process. Examples include the hydride abstraction of alkanes in methane chemical ionization. In methane CI, both CH_5^+ and $C_2H_5^+$ are capable of hydride abstraction. These species have large hydride-ion affinities, which results in the loss of H^- for long-chain alkanes, according to the general reaction

$$R^+ + M \rightarrow [M-H]^+ + RH$$

For methane, R^+ is CH_5^+ and $C_2H_5^+$, and M is a long-chain alkane. In the case of CH_5^+, the reaction proceeds to form $[M-H]^+ + CH_4 + H_2$. The spectra resulting from hydride abstraction will show an M–1 *m/z* peak resulting from the loss of H^-. This reaction is exothermic so fragmentation of the $[M-H]^+$ ion is often observed.

Often, both hydride-abstraction and proton-transfer ionization can be evident in the sample spectrum. One example is the methane CI spectrum of long-chain methyl esters, where both hydride abstraction from the hydrocarbon chain and proton transfer to the ester function occur. In the methane PCI spectrum of methyl stearate, for example, the MH^+ peak at *m/z* 299 is created by proton transfer and the $[M-1]^+$ peak at *m/z* 297 is created by hydride abstraction.

Addition

For many analytes, proton-transfer and hydride-abstraction chemical ionization reactions are not thermodynamically favorable. In these cases, reagent gas ions are often reactive enough to combine with the analyte molecules by condensation or association (addition reactions). The resulting ions are called adduct ions. Adduct ions are observed in methane chemical ionization by the presence of $[M+C_2H_5]^+$ and $[M+C_3H_5]^+$ ions, which result in M+29 and M+41 *m/z* mass peaks.

Addition reactions are particularly important in ammonia CI. Because the NH_3 has a high proton affinity, few organic compounds will undergo proton transfer with ammonia reagent gas. In ammonia CI, a series of ion-molecule reactions takes place, resulting in the formation of NH_4^+, $[NH_4NH_3]^+$, and $[NH_4(NH_3)_2]^+$. In particular, the ammonium ion, NH_4^+, will give rise to an intense $[M+NH_4]^+$ ion observed at M+18 *m/z*, either through condensation or association. If this resulting ion is unstable, subsequent fragmentation may be observed. The neutral loss of H_2O or NH_3, observed as a subsequent loss of 18 or 17 *m/z*, respectively, is also common.

Charge exchange

Charge-exchange ionization can be described by the reaction:

$$X^{+\bullet} + M \rightarrow M^{+\bullet} + X$$

where X^+ is the ionized reagent gas and M is the analyte of interest. Examples of reagent gases used for charge exchange ionization include the noble gases (helium, neon, argon, krypton, xenon, and radon), nitrogen, carbon dioxide, carbon monoxide, hydrogen, and other gases that do not react “chemically” with the analyte. Each of these reagent gases, once ionized, has a recombination energy expressed as:

$$X^{+\bullet} + e^{-} \rightarrow X$$

or simply the recombination of the ionized reagent with an electron to form a neutral species. If this energy is greater than the energy required to remove an electron from the analyte, then the first reaction above is exothermic and thermodynamically allowed.

Charge-exchange chemical ionization is not widely used for general analytical applications. It can, however, be used in some cases when other chemical ionization processes are not thermodynamically favored.

Negative CI Theory

Negative chemical ionization (NCI) is performed with analyzer voltage polarities reversed to select negative ions. There are several chemical mechanisms for NCI. Not all mechanisms provide the dramatic increases in sensitivity often associated with NCI. The four most common mechanisms (reactions) are:

- Electron capture
- Dissociative electron capture
- Ion pair formation
- Ion-molecule reactions

In all of the cases except the ion-molecule reactions, the reagent gas serves a function different from the function it serves in PCI. In NCI, the reagent gas is often referred to as the buffer gas. When the reagent gas is bombarded with high energy electrons from the filament, the following reaction occurs:

$$\text{Reagent gas} + e^-_{(230\text{eV})} \rightarrow \text{Reagent ions} + e^-_{(\text{thermal})}$$

If the reagent gas is methane (Figure 2), the reaction is:

$$CH_4 + e^-_{(230\text{eV})} \rightarrow CH_4^+ + 2e^-_{(\text{thermal})}$$

The thermal electrons have lower energy levels than the electrons from the filament. It is these thermal electrons that react with the sample molecules.

There are no negative reagent gas ions formed. This prevents the kind of background that is seen in PCI mode and is the reason for the much lower detection limits of NCI. The products of NCI can only be detected when the MS is operating in negative ion mode. This operating mode reverses the polarity of all the analyzer voltages.

Carbon dioxide is often used as a buffer gas in NCI. It has obvious cost, availability, and safety advantages over other gases.

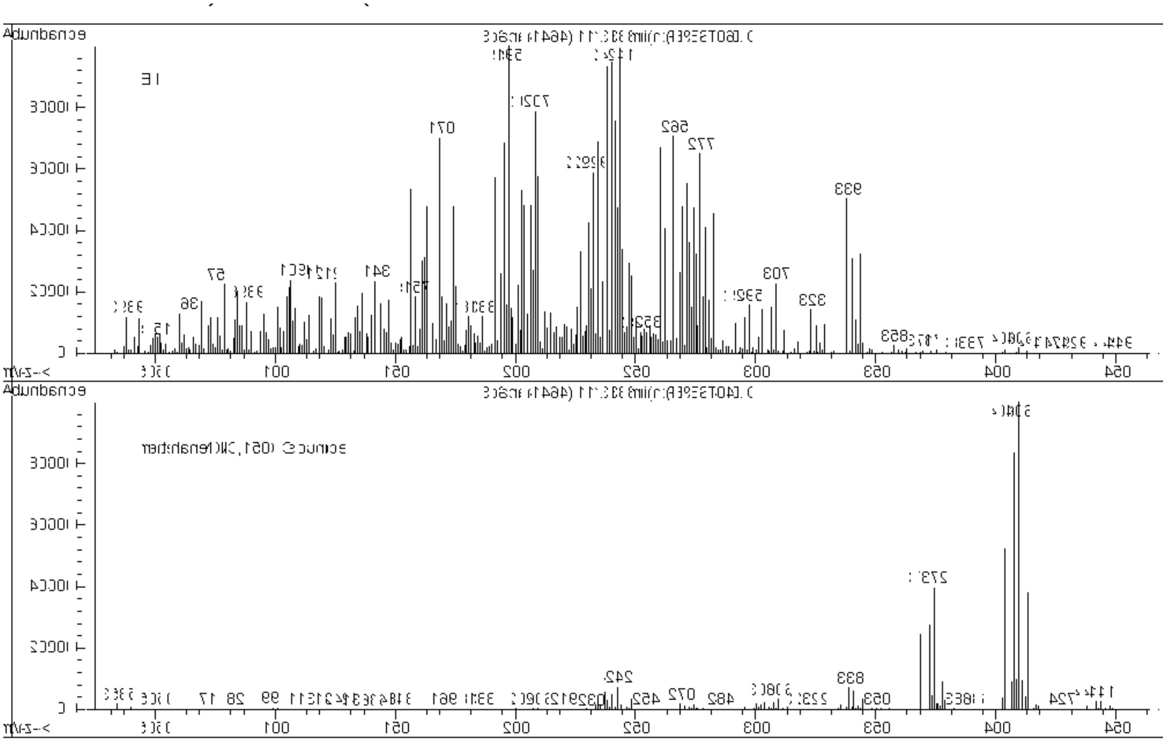


Figure 2 Endosulfan I (MW = 404): EI and methane NCI

Electron capture

Electron capture is the primary mechanism of interest in NCI. Electron capture (often referred to as high-pressure electron capture mass spectrometry or HPECMS) provides the high sensitivity for which NCI is known. For some samples under ideal conditions, electron capture can provide sensitivity as much as 10 to 1000 times higher than positive ionization.

Note that all the reactions associated with positive CI will also occur in NCI mode, usually with contaminants. The positive ions formed do not leave the ion source because of the reversed lens voltages, and their presence can quench the electron capture reaction.

The electron capture reaction is described by:

$$MX + e^{-}_{\text{(thermal)}} \rightarrow MX^{-\bullet}$$

where MX is the sample molecule and the electron is a thermal (slow) electron generated by the interaction between high energy electrons and the reagent gas.

In some cases, the $MX^{-\bullet}$ radical anion is not stable. In those cases the reverse reaction can occur:

$$MX^{-\bullet} \rightarrow MX + e^{-}$$

The reverse reaction is sometimes called autodetachment. This reverse reaction generally occurs very quickly. Thus, there is little time for the unstable anion to be stabilized through collisions or other reactions.

Electron capture is most favorable for molecules that have hetero-atoms. For example: nitrogen, oxygen, phosphorus, sulfur, silicon, and especially the halogens: fluorine, chlorine, bromine, and iodine.

The presence of oxygen, water, or almost any other contaminant interferes with the electron-attachment reaction. Contaminants cause the negative ion to be formed by the slower ion-molecule reaction. This generally results in less sensitivity. All potential contamination sources, especially oxygen (air) and water sources, must be minimized.

Dissociative electron capture

Dissociative electron capture is also known as dissociative resonance capture. It is a process similar to electron capture. The difference is that during the reaction, the sample molecule fragments or dissociates. The result is typically an anion and a neutral radical. Dissociative electron capture is illustrated by the reaction equation:

$$MX + e^{-}_{(\text{thermal})} \rightarrow M^{\bullet} + X^{-}$$

This reaction does not yield the same sensitivity as electron capture, and the mass spectra generated typically have lower abundance of the molecular ion.

As with electron capture, the products of dissociative electron capture are not always stable. The reverse reaction sometimes occurs. This reverse reaction is sometimes called an associative detachment reaction. The equation for the reverse reaction is:

$$M^{\bullet} + X^{-} \rightarrow MX + e^{-}$$

Ion pair formation

Ion pair formation is superficially similar to dissociative electron capture. The ion pair formation reaction is represented by the equation:

$$MX + e^{-}_{(\text{thermal})} \rightarrow M^{+} + X^{-} + e^{-}$$

As with dissociative electron capture, the sample molecule fragments. Unlike dissociative electron capture however, the electron is not captured by the fragments. Instead, the sample molecule fragments in such a way that the electrons are distributed unevenly and positive and negative ions are generated.

Ion-molecule reactions

Ion-molecule reactions occur when oxygen, water, and other contaminants are present in the CI ion source. Ion-molecule reactions are two to four times slower than electron-attachment reactions and do not provide the high sensitivity associated with electron capture reactions. Ion-molecule reactions can be described by the general equation:

$$M + X^- \rightarrow MX^-$$

where X^- is most often a halogen or hydroxyl group that was created by ionization of contaminants by electrons from the filament. Ion-molecule reactions compete with electron capture reactions. The more ion-molecule reactions that occur, the fewer electron capture reactions occur.

Single Quadrupole MS Operation

Understanding the operation of a singlequadrupole provides insight into some of the features of a 7200 Q-TOF GC/MS system. This section reviews the fundamentals of a single quadrupople mass spectrometer.

Mass spectrometry is based on the analysis of ions moving through a vacuum.

As described in the previous section, the ionization of a sample occurs in the ion source. The ions are filtered by a mass analyzer that controls the motion of the ions as they travel out of the analyzer. In the case of a single quadrupole MS, the ions will travel to the detector to be converted into actual signals (Figure 3). In Q-TOF MS, however, the filtered ions are sent to a time-of-flight tube prior to detection.

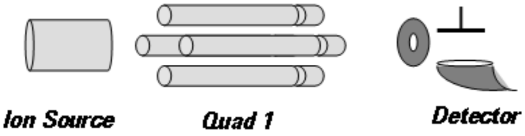


Figure 3 Schematic for single quadrupole mass spectrometer

The quadrupole mass analyzer consists of four parallel rods to which specific DC and RF voltages are applied. These rods filter out all ions except those of one or more particular *m/z*, or mass to charge ratio value as determined by the voltages applied.

The RF is applied to all four rods, but the negative (–) rods are 180 degrees out of phase with the positive (+) rods. The rods are labeled + and – in reference to the DC voltages applied to them.

All ions that comprise the sample are generated at the source. However, when a specific set of voltages is applied, only ions of the corresponding *m/z* value may pass through the quadrupole to reach a detector, in this case, the flight tube. As the voltages are increased to other values, ions with other *m/z* values are allowed to pass through. A full MS scan is obtained by increasing the DC and RF voltages applied to the four rods over an expanded range of values.

A conceptual model can be used to explain the theory of a single quadrupole mass spectrometer. See Figure 4.

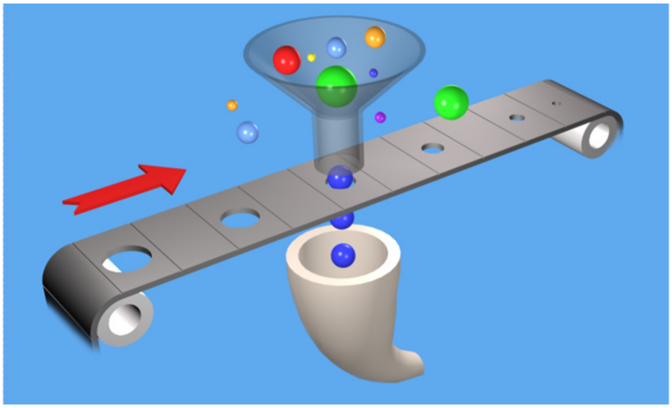


Figure 4 Conceptual model of a single quadrupole mass spectrometer

In the model,

- All of the ions contained in a sample are formed in the external ionization source and collected in a funnel. The balls of different colors and sizes represent different ions having different *m/z* values.
- The quadrupole mass analyzer is represented by a moving belt that serves to filter the ions as they pass through openings of various sizes. The ions pass from the funnel, through the filter, and are fragmented and focused before they are sent to the flight tube.
- The collecting funnel below the filtering belt represents the focusing electronics prior to the flight tube.

As the belt (the analyzer) moves, or the voltages on the rods are changed, ions with different *m/z* values are filtered through the mass spectrometer.

As the analyzer moves from a small *m/z* value to increasingly larger values, a full MS scan is created.

If the belt does not move, the detector continues to monitor the same single *m/z* value over the entire scan period. This type of analysis is known as selected ion monitoring, or SIM. It is the most sensitive operating mode for a single quadrupole mass spectrometer.

The scan period is selected (fixed) by the user. The user may set the scan to a specific mass range (for example, *m/z* 50 to 1000) *or* to dwell on one selected ion (SIM) *or* to dwell on several selected ions during the scan period. The quadrupole mass filter is not scanned over a range in the SIM mode. The required RF/DC voltages are set to filter a single mass for a specified dwell time before moving to the setting for the next SIM.

The ions that pass through the quadrupole can either be measured by a detector, or sent through additional filtering methods for MS/MS analysis.

Ion fragmention and collision cell technology

As charged ions move through the analyzer chamber, they can collide with each other and with the gas molecules present throughout the region. When the voltages increase along their path, ions have more translational energy, which causes fragmentation as they collide.

Because fragmentation patterns provide information about the the original ions, a collision cell can be used to purposely fragment the ions that pass through the analyzer. These ions are called precursor ions, and their fragments are called product ions. The quadrupole can be tuned to select which precursor ion travels to the collision cell. Analysis of their product ions by the detector in the flight tube provides more accurate mass measurement.

Different types of collision cells can be used. The cell can be another quadrupole, a hexapole (six rods like the one used in the 7200 Q-TOF), an octopole (eight rods), or even a transverse wave guide. Whichever geometry is used, an inert, nonreactive gas is required for use as the collision gas. In addition, the voltages applied to the collision cell must be different from those applied to the quadrupoles to accelerate the movement of all of the ions so that their collision energy is sufficient to cause fragmentation.

In the collision cell, a potential difference is always present. This ensures that the precursor ions coming from the quadrupole or fragment ions generated in the collision cell are transmitted and not allowed to drift around at random, which helps to focus the ion stream before it is sent to the detector.

The use of a collision cell helps to eliminate crosstalk, which occurs when product ions from a previously selected precursor appear in a product ion spectrum of a subsequently selected precursor because of slow clearance from the collision cell. This creates a composite product ion spectrum, which can be difficult to interpret.

Time-of-Flight MS Operation

The previous section discusses the theory behind ion separation using quadrupole mass spectrometry, and fragmentation with a collision cell. In quadrupole time-of-flight mass spectrometry, these methods are used for preliminary ion separation prior to detection at the end of the flight tube.

Time-of-flight mass spectrometry measures the time it takes for ions to travel a known distance, and using this time value, determines the mass to charge ratio of the ions.

Ions are accelerated through a flight tube by an electric field of known strength. This acceleration results in an ion having the same kinetic energy as any other ion that has the same charge. The velocity of the ion depends on the mass-to-charge ratio. The time that it subsequently takes for the particle to reach a detector at a known distance can be measured. This time will depend on the mass-to-charge ratio of the particle (heavier particles reach lower speeds). From this time and the known experimental parameters, one can find the mass-to-charge ratio of the ion using the following relationships:

$KE = 1/2\ m\ v^{2}$

$v = d/t$

$t = m^{1/2\,*}\ d/(2KE)^{1/2}$

We can assume that the d/2KE term of the above equation remains constant. Therefore, the mass of the particle can be determined by measuring the time the particle takes to travel the flight tube.

Consider the Q-TOF model in Figure 5. Ions that have been selected in the quadrupole, and fragmented in the collision cell are sent to the flight tube, where they are sent in an orthogonal direction up the tube. This means that they are sent in a direction perpendicular to their flight through the quadrupole and collision cell. The orthogonal direction minimizes the effects of ion generation and transmission on mass measurement because any unwanted ions are pushed or ejected from the direction of travel by pulsed voltages applied onto deflection plates.

The nearly parallel beam of ions passes into the time- of- flight ion pulser. The ion pulser is a stack of plates, each one (except the back plate) with a center hole. The ions pass into this stack from the side just between the back plate and the first plate with its center hole. To start the flight of the ions to the detector, a high voltage (HV) pulse is applied to the back plate. The applied pulse accelerates the ions through the stack of pulser plates, acting as a rapid- fire ion gun.

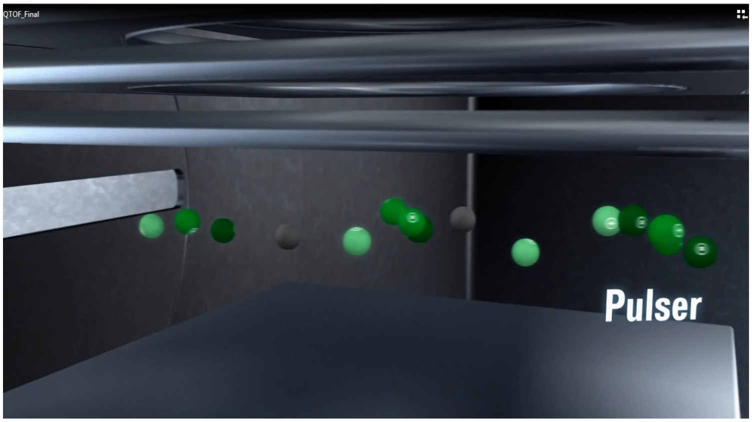


Figure 5 Ions are attracted and repelled by the pulser

The charged plates of the pulser send the charged ions through the flight tube, which is about one meter in length (Figure 6). Changes in temperature and humidity can alter pulse electronics. In addition, any collision of an ion with residual gas slows the ion on its path to the detector and affects the accuracy of the mass calculation. Therefore, the flight tube should be maintained at constant temperature and vacuum.

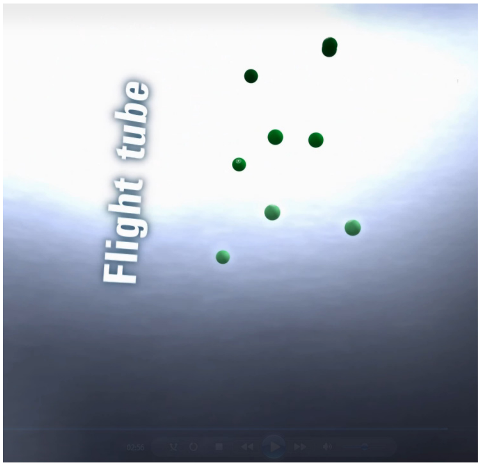


Figure 6 Ions travel up the flight tube in a direction orthogonal to their entrance

Once through the flight tube, the particles must be counted in some way. They are sent back down the tube to a detector by reflection from a dual-stage charged mirror (Figure 7). Since two ions of the same mass may leave the pulser at different positions, or they may have different kinetic energies, the mirror helps to minimize the effect these conditions may have on flight time. Ions with higher kinetic energy will penetrate further into the ion mirror, causing them to travel a further distance. This equalizes the arrival time of the ions to the detector.

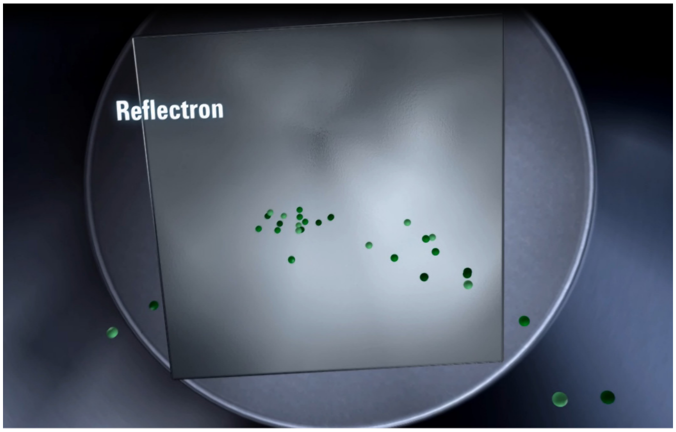


Figure 7 Ion reflect off the dual stage ion mirror

The ions enter the ion pulser with a certain amount of forward momentum orthogonal to the flight direction in the flight tube. Therefore, when they reflect off the mirror, they never return to the ion pulser, but move to where the ion detector is mounted. (Figure 8)

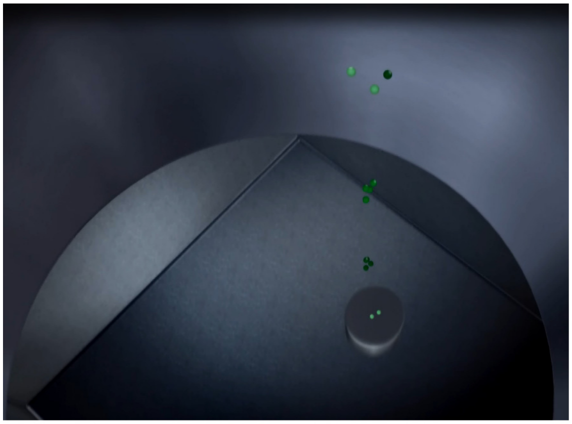


Figure 8 Ions travel down the flight tube toward the detector

At the surface of the ion detector is a microchannel plate (MCP), which is a very thin plate containing a set of microscopic tubes that pass from the front surface to the rear of the plate. This is shown in Figure 9. When an ion hits the front surface of the MCP, an electron escapes and begins the process of electrical signal amplification. As freed electrons collide with the walls of the microscopic tubes, an ever-increasing cascade of electrons travels to the rear of the plate. Roughly 10 times more electrons exit the MCP than incoming ions contact the surface.

These electrons are then focused onto a scintillator, which, when struck by electrons, produces a flash of light. The light from the scintillator is focused through two small lenses onto a photomultiplier tube (PMT), which produces the electrical signal read by the data system. The reason for producing an optical signal from the MCP electrons is because the output of the MCP is at roughly - 6000 volts. The light produced by the scintillator passes to the PMT, which has a signal output at ground potential.

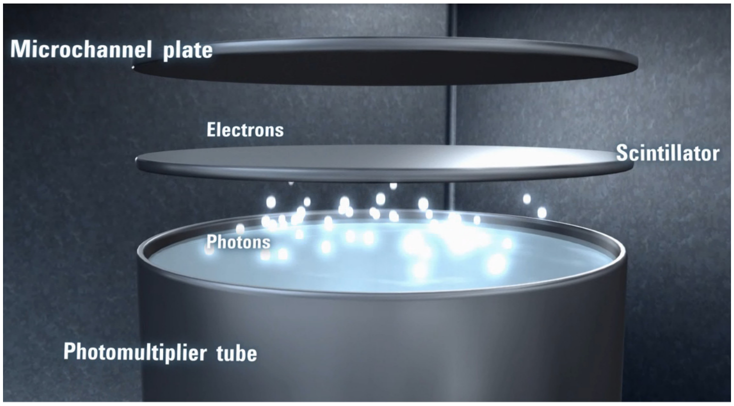


Figure 9 Ion send a signal as they hit the detetctor

With analog to digital conversion, the detector can count more than one ion at a time. The detector records the time and number of ions as they arrive. (Figure 10).

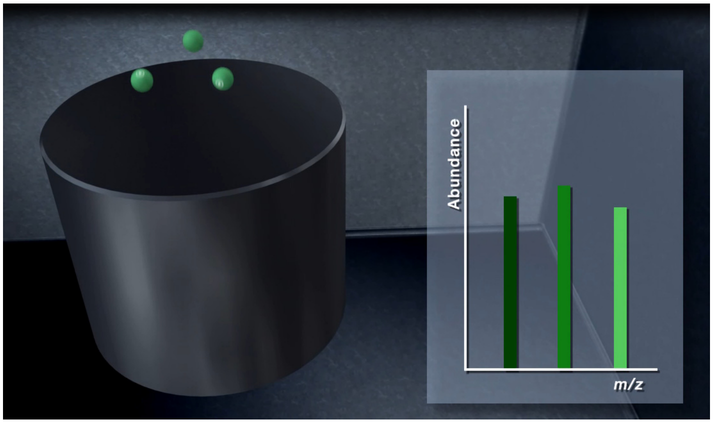


Figure 10 Detector records the time and number of ions as they exit the flight tube

Quadrupole Time-of-Flight MS Operation

The previous sections regarding ionization, and the operation of a single quadrupole mass spectrometer, collision cell, and time-of-flight mass spectrometry help to clarify the principles of Q-TOF operation. This section explains how the technologies work together to perform accurate mass detection.

Design of the 7200-Q-TOF

The Agilent 7200 Accurate-Mass Quadrupole Time-of-Flight GC/MS consists of an ion source, followed by ion optics that transfer the ions to the first quadrupole positioned to the right of it. A diagram of the current 7200 Q-TOF mass spec is shown in Figure 11.

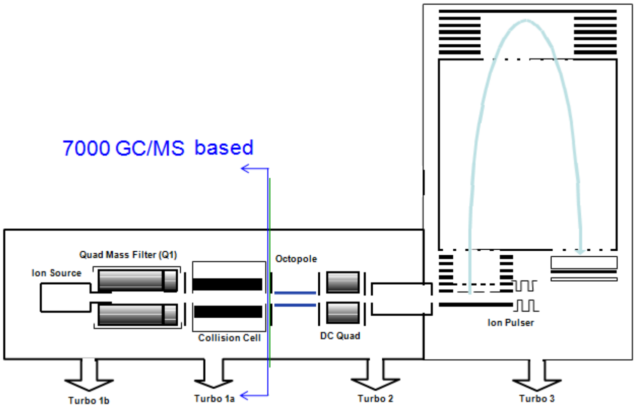


Figure 11 The 7200 Q-TOF Overview

In the quadrupole, selected ions are filtered. The filtered ions then enter a collision cell where they are fragmented. The collision cell is geometrically a hexapole filled with nitrogen as the collision gas.

The fragment ions formed in the collision cell are then sent through a slicer, which is an electrically charged slot between the collision cell and the entrance to the flight tube. The slicer is used to focus and further separate the ions prior to entering the flight tube.

Once through the slicer, the selected ion are propelled through the flight tube by the pulser. The ions are sent in a direction orthogonal to their entrance into the flight tube. This ensures that once the ions hit the mirror at the top of the flight tube, they reflect off in the direction of the detector, instead of back toward the pulser.

The flight tube is 1 meter in length, providing a 2-meter flight path after the ions reflect off the mirror. The dual-stage ion mirror helps to minimize variations in flight time, correcting for the fact that the ions do not start in the same plane in space relative to flight direction.

An analog to digital detector at the bottom of the flight tube records the time and abundance of the ions as they hit the detector plates.

Innovative features in the 7200 Q-TOF

The most innovative feature of the Agilent Accurate-Mass Q-TOF GC/MS is the Removable Ion Source (RIS) technology. The features of the new ion source design allows the fast and complete swapping of the source, including filaments, in less than 30 minutes without venting.

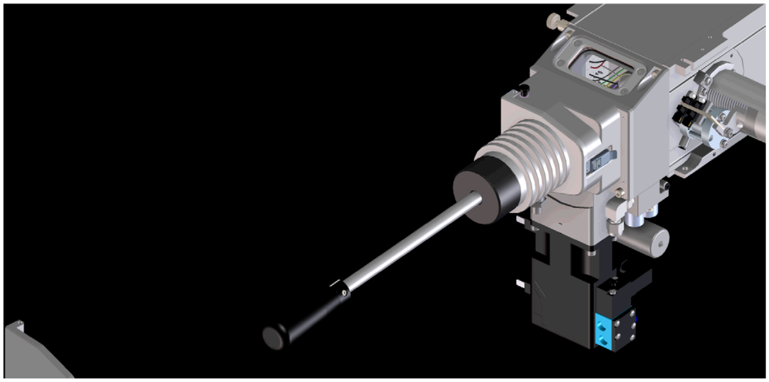


Figure 12 Removable Ion Source

The RIS probe design consists of a bayonet that attaches to the source for removing and replacing it in the analyzer chamber. At the other end of the RIS probe is a cooling chamber (Figure 13). The bayonet retracts and extends, moving the source into and out of the cooling chamber during removal or installation.

When the RIS probe assembly is attached to the front of the MS, replacing the RIS cover door, an automatic pneumatic gate valve closes off the MS system from the RIS cooling chamber, maintaining the MS at operational temperature and vacuum while the RIS cooling chamber is attached. The RIS cooling chamber can then be flushed with dry nitrogen, eliminating the chamber of oxygen, moisture and other contaminants prior to the source's removal from the MS and entry into the cooling chamber.

After the nitrogen purge and pumping down of the chamber, the gate valve automatically opens to allow the bayonet to reach the source, while the transfer line automatically retracts, releasing the source body from the transfer line to avoid damage. The bayonet can then be used to pull the source from the MS into the cooling chamber. The gate valve again closes the cooling chamber off from the system. The source can be cooled within

10 minutes to a safe temperature, then replaced using the RIS probe. This eliminates the necessity of venting the instrument, and pumping down prior to the next run, saving cycle time.

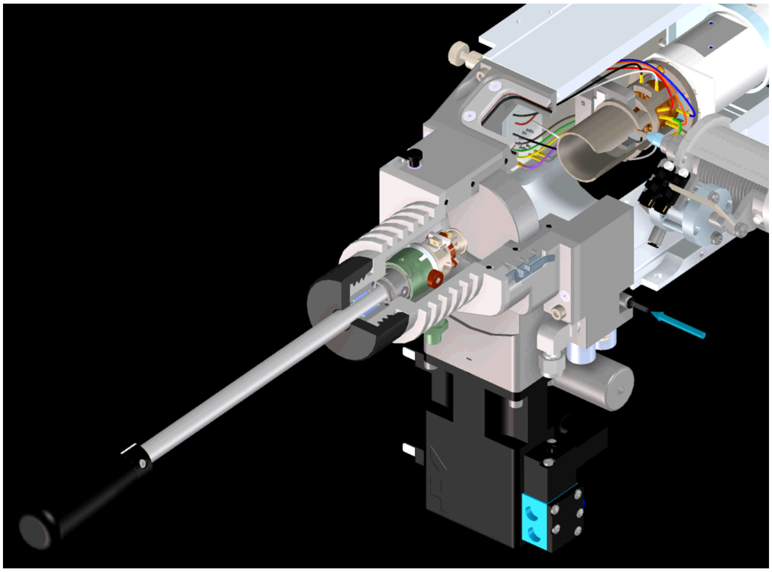


Figure 13 Internal view of RIS system

Another innovative feature of the 7200 Q-TOF GC/MS is the proprietary Internal Reference Mass (IRM) delivery system. The use of an internal reference mass helps to “lock” the mass axis for each scan during a calibration. The 7200 Q-TOF can deliver the IRM to the source at low or high concentrations for “on the fly” mass corrections. This provides easy and reliable mass accuracy for a wide range of mass detection.

The quadrupole and collision cell designs are also innovative features. The hot, quartz monolitihic analyzer and collision cell are identical to those in the 7000 Triple Quad GC/MS. A post filter focuses the ion beam exiting the quadrupole, which ensures effective concentration of the ions exiting the quad.

The collision cell is actually a hexapole filled with a nitrogen gas stream. Agilent innovation has led to the design of a collision cell that has axial acceleration for high speed MS/MS analysis. The collision cell accelerates the fragmented product ions through the MS, enabling faster generation of high quality MS/MS spectra without cross-talk.

The proprietary time-of-flight tube design is another innovative feature. The INVAR flight tube is sealed in a vacuum-insulated shell. This design eliminates thermal mass drift from temperature changes, and helps to maintain mass accuracy.

Agilent’s high speed electronics is another innovation in Q-TOF technology. The 7200 Q-TOF features 4GHz ADC electronics that provide a high sampling rate of 32 Gbit/s. This improves resolution, mass accuracy, and sensitivity for low-abundance samples. In addition, dual gain amplifiers can process detector signals simultaneously though low and high-gain channels, which extends the dynamic range to 10^5.

3

Agilent 7200 Accurate-Mass Q-TOF and Performance

This chapter shows how the Agilent 7200 Accurate-Mass Q-TOF GC/MS reduces chemical and electronic noise and how each component contributes to enhanced instrument performance.

How the 7200 Q-TOF Meets Performance Measures

There are several performance standards for the 7200 Q-TOF GC/MS. The most important are:

- Resolving Power
- Mass Accuracy
- Scan Speed
- Sensitivity
- Dynamic Range

Resolving Power

Resolving power in mass spectrometry refers to the ability to distinguish between two peaks of slightly different mass to charge ratios (*m/z*) in a mass spectrum. High resolving power enables improved mass measurement accuracy and charge state identification of multiply charged ions, which leads to better compound identification. The vacuum-insulated flight tube and dual stage ion mirror in the 7200 Q-TOF GC/MS provides consistently high resolution.

Mass Accuracy

Mass accuracy is the ability with which the analyzer can accurately provide *m/z* information. In mass spectrometry, this is a function of stability and resolution. This performance standard is important because accurate mass detection reduces the risk of effort invested on the wrong molecule. The high sampling rate and multiple ion event data provided by the 4GHz analog to digital electronics lead to highly accurate mass identification.

Scan Speed

The scan rate of a mass spectrometer refers to how fast it scans a mass spectrum. This is important for chromatography applications where the entire mass spectrum must be scanned faster than the elution time of the chromatographic peak. Ideally, a minimum of ten complete mass spectra are acquired for a single chromatographic peak. The fast electronics of the 7200 Q-TOF has a data acquisition rate of about 10,000 pulses per second. Each pulse can contain up to 100,000 data points. This pulsed data can develop an entire mass spectrum from a single pulse of ions. This provides a spectrum with excellent ion statistics.

Sensitivity

Sensitivity in MS data is affected by detection limits, sample dilution, and sample contamination. Improvements in MS sensitivity are made through increased signal strength and a reduction in chemical noise. The design of 7200 Q-TOF GC/MS has improved sensitivity with new removable ion source design that features a high sensitivity extractor lens and new method of source exchange that minimizes the risk of contamination in the instrument. In addition, the high separation, focusing and fragmentation levels achieved by the quadrupole and collision cells, as well as the elimination of contaminants prior to the flight tube by the slicer and pumping systems help to contribute to the high sensitivity of the 7200 Q-TOF GC/MS.

Dynamic Range

Dynamic range is a measure of the detection range of a detector because it describes the range over which accurate masses can be determined. It is the ratio of the largest to smallest detectable signal. The analog to digital detection of the 7200 Q-TOF provides 4-5 orders magnitude dynamic range, and 32 Gbit/sec of information during a run.

7200 Accurate-Mass Q-TOF Design

In the design of the 7200 Q-TOF GC/MS, the performance measures were addressed within all stages of instrumentation, from the ion source to the detector.

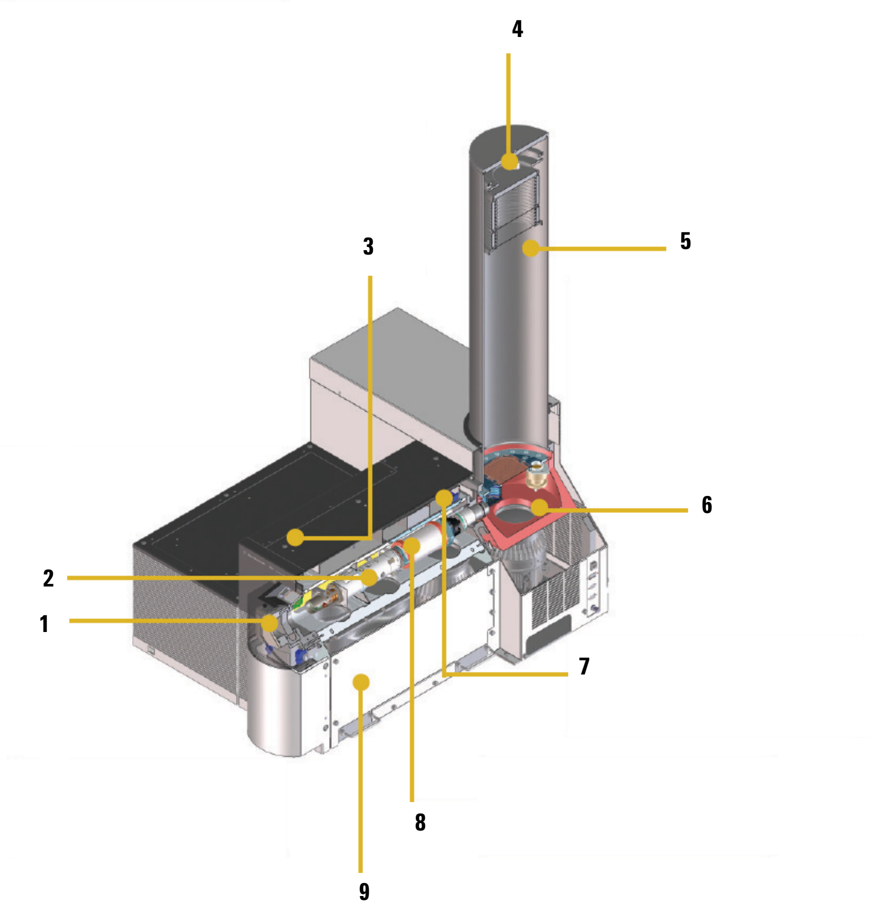


Figure 14 7200 Q-TOF and Performance

1. RIS includes repeller, ion volume, high sensitivity extraction lens and filaments for easy source exchange with minimal downtime and contamination.
2. Analyzer uses hyperbolic quadrupoles to optimize ion transmission and spectral resolution.
3. ADC electronics provide high sampling rates, improving resolution, mass accuracy, and sensitivity for low abundance samples.
4. Dual stage ion mirror improves second-order time focusing in the flight tube by extending the ion flight time provides high mass resolution.
5. Proprietary INVAR flight tube is vacuum-insulated and eliminates thermal mass drift from temperature changes, providing high mass accuracy and resolution.
6. Analog to digital detector can record multiple ion events, which provides accurate mass readings, wide mass ranges, and wide range of concentrations.
7. Internal reference mass flow control system can deliver the compound to the source at low or high concentrations during the run, allowing accurate calibrations at wide mass ranges.
8. High pressure collision cell with linear acceleration optimizes MS/MS fragmentation while eliminating crosstalk, even at very low dwell times. A small diameter high frequency hexapole assembly assists with capturing and focusing fragmented ions.
9. Vacuum system incorporating the use of three turbomolecular pumps efficiently eliminates neutral materials prior to the detector

How each Component Works to Meet Performance Measures

This section describes in more detail how each of the components of the 7200 Q-TOF contributes to high sensitivity, accurate mass deteiction, and high mass resolution.

Removable Ion Source

The 7200 Q-TOF uses the same front end ionization methods as Agilent single and triple quadrupole mass spectrometers. However, this technology has been improved with the new removable ion source.

The EI ion source operates by electron impact ionization and the CI ion source operates by chemical ionization. Sample ions enter the source through the GC/MS interface. The sample is ionized in the ionization chamber, which is made up of the source body, repeller and drawout plate.

A filament attached to the source body emits electrons into the ionization chamber through the guidance of a magnetic field. These electrons interact with sample molecules, ionizing and fragmenting them. The EI ionization source in the 7200 Q-TOF contains two filaments, which allows for a choice of filament depending upon tuning results.

Once the sample has been ionized, the ions are directed by the repeller through a stack of electrostatic lenses. The repeller contains a positive voltage, which pushes positive ions into the lens stack. There the ions are concentrated into a tight beam and pushed into the analyzer. Slots in the source body allow the vacuum system to pump away ions of carrier gas and unionized material as the sample ions enter the quad, thereby reducing neutral noise and improving sensitivity.

The removable ion source technology allows source removal and replacement with the use of an RIS probe and bayonet. The source wiring is permanently fixed inside the analyzer chamber, providing quick and easy source installation from outside the analyzer chamber. The use of the bayonet eliminates the need to open the analyzer chamber, allowing air and moisture in to the MS during installation. This reduces contamination in the instrument, helping to reduce background noise.

Quad mass filter

The quadrupoles consist of hyperbolic rods that optimize ion transmission and spectral resolution. The quadrupole configuration tends to generate less ion loss than circular rods. The gold plated quartz material allows the analyzer to operate at high temperatures and low vacuum, eliminating the contamination that occurs with lower temperatures.

Pre- and post-filter

The end section of the quadrupole assembly also consists of short hyperbolic rods, but their RF voltages are only high enough to guide ions into the collision cell. A similar set of rods is found on the exit side of the collision cell. These short RF-only rods act as filters to ensure optimum ion transmission in and out of the collision cell.

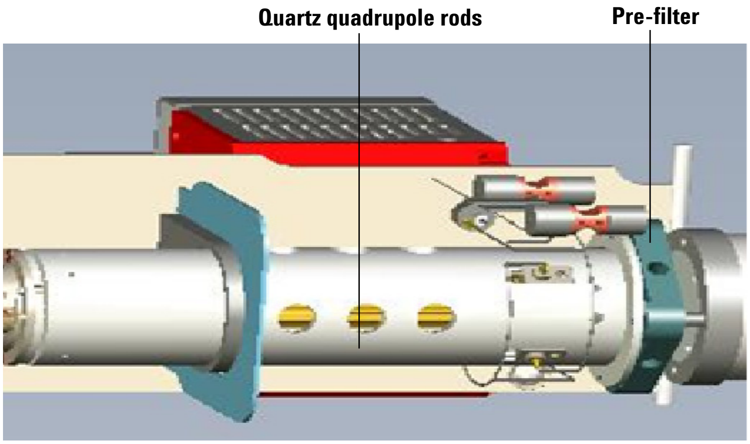


Figure 15 Quadrupole assembly

Collision cell

What is the collision cell?

The collision collects parents of precursor ions and ion fragments, thermalizes the ion beam, and focuses the beam into the flight tube. The collision cell is a high pressure hexapole assembly with its linear acceleration adjusted to optimize MS/MS fragmentation while eliminating crosstalk even at very low dwell times .

The components that contribute to this higher sensitivity and faster response are

- Small diameter hexapole collision cell
- High frequency hexapole collision cell
- Linear axial acceleration
- High pressure collision cell
- High speed digital electronics

The collision cell contains nitrogen, which is eliminated by the vacuum pump along with carrier gas and unfragmented sample ions. The small diameter of the hexapole assembly assists in colliding fragmented ions.

Why a hexapole?

The geometry of a hexapole provides advantages in two domains: ion focusing and ion transmission (Figure 16).

- The first advantage is in ion focusing. Studies have shown that a quadrupole provides better ion focusing than a hexapole and a hexapole provides better ion focusing than an octapole. Therefore, ion focusing improves with a lower number of poles in the filter.
- The second advantage involves ion transmission across a wide mass range, or *m/z* bandwidth. In this case, the octapole is better than the hexapole, which is better than the quadrupole.

The hexapole is chosen after extensive modeling, simulation and experimentation because it offers the best compromise between the focusing of a quadrupole and the ion transmission of an octapole.

Collision cell design

The collision cell hexapole consists of six resistively coated rods used to generate a 5V potential difference across the length of the collision cell (Figure 16).

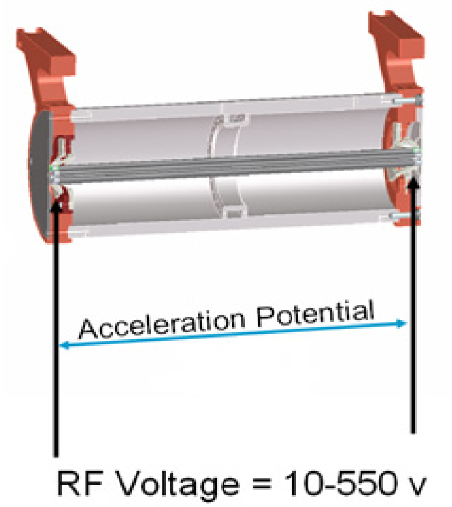


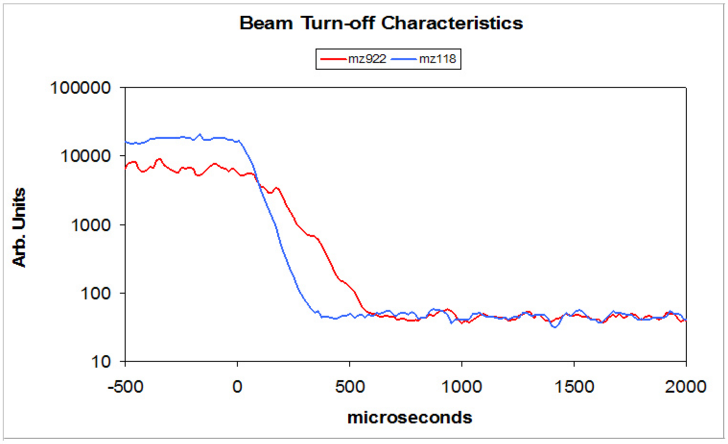
Figure 16 Collision cell design

A potential difference is always present. This ensures that the precursor ions coming from the quadrupole, or fragment ions generated in the collision cell, are transmitted and not allowed to drift around at random.

Sweeping out the ions in this manner avoids the issue of crosstalk where residual product ions from a previous experiment can interfere with the product ion spectrum of a subsequent experiment (see Figure 17). A collision energy voltage is applied over the accelerating linear voltage to generate fragments or product ions.

Length of time for collision cell flushing

The low degree of crosstalk can be demonstrated by examining how long it takes to evacuate ions from the collision cell (Figure 17).



0 V Collision Energy 5 V Applied Axial Potential

Figure 17 Collision cell clearing profile (500 pg Alprazolam, 20 ms dwell time)

The figure shows that the higher the mass the longer it takes to evacuate the collision cell. For example, *m/z* 922 takes about 600 µsec to evacuate the collision cell using the linear potential, while *m/z* 118 only takes 350 µsec. This also demonstrates the low degree of crosstalk since the Y axis is logarithmic, showing complete clearance of the cell. This means that an inter-scan delay of 5 msec will be more than adequate to flush the collision cell of all ions.

Proprietary INVAR flight tube

The 7200 Q-TOF flight tube is about 1 meter in length and maintains vacuum pressure of about 10^{-7} torr. It is vacuum insulated throughout the length of the tube. This eliminates the ion scatter that can occur at higher pressures, and the temperature fluctuations that can change the flight distance of the ions. In addition, changes in temperature and humidity can change flight distance. The insulated flight tube helps minimze these effects, and increase measurement accuracy.

At the entrance of the flight tube is a slicer, which is a narrow lens that refocuses the ions so that they will enter the time of flight analyzer as a parallel beam. This helps minimize variability in measurement that occurs because ions that do not start in the same plane in space relative to flight direction.

The dual stage ion “mirror” at the end of the flight tube reflects the ions that arrive near the end of the flight tube towards the detector. As it reflects, it refocuses the ions and minimizes the kinetic energy variations in arrival time. Ions with higher kinetic energies will penetrate further into the mirror, traveling a greater distance, helping them to reach the detector simultaneously. This corrects the variability in measurement and results in higher resolving power.

Analog-to-digital detector

The analog to digital detector records the time and number of ions arriving at the detector. Fast electronics allow high sampling rates, and many data points in each pulse of the detector. Sample concentration does not impact arrival time, so this detector provides data for a wider dynamic range of sample concentrations. In addition, this detector does not drop ions or suffer from “dead time”effects.

Pumping system

The vacuum system is a five-stage pumping system created by one split flow and two additional turbomolecular pumps that are backed up by a single roughing (mechanical) pump (Figure 18). The vacuum system removes particles of carrier gas and any unionized molecules from the ion source outlet, the collision cell and the analyzer. In addition, it creates the constant low pressures necessary to focus the ions and propel them through the 1-meter flight tube with minimal ion scatter.

The efficiency of the vaccum affects the mass accuracy, and resolution of the detector because ion collisions with residual gas can alter the flight time of the ion. Accurate mass calculation depends upon accurate flight times. Therefore, the background gas pressure in the flight tube is very low and very consistant.

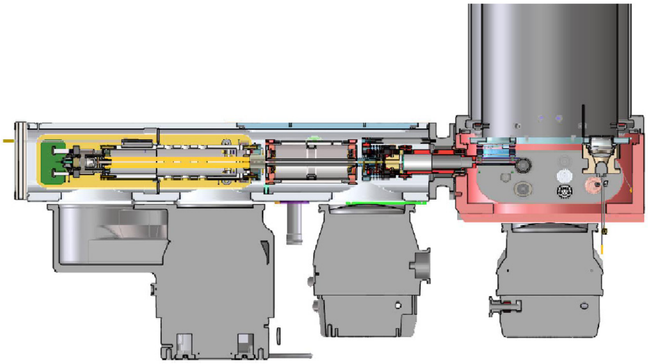


Figure 18 Vacuum system

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