PRODUCT

INFORMATION

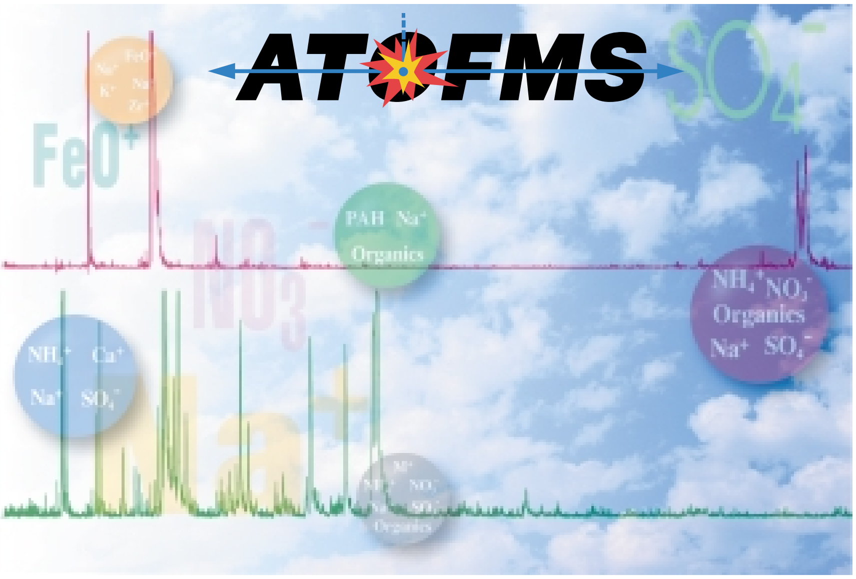
Model 3800 Aerosol Time-of-Flight Mass Spectrometer

TSI Incorporated's Aerosol Time-of-Flight Mass Spectrometer (ATOFMS) is the first commercial instrument to offer the ability to determine the size and chemical composition of individual aerosol particles in near real time! It characterizes short-lived and dynamic processes in a number of applications and, therefore, avoids artifacts associated with traditional sampling and analysis methods. That's why the ATOFMS is expected to usher in an exciting new era of particle research and measurement.

The Model 3800 Aerosol Time-of-Flight Mass Spectrometer (ATOFMS) is a revolutionary instrument in the field of analytical chemistry, and it offers great potential in areas such as atmospheric science, biological detection, and pharmaceutical manufacturing. Based on an instrument built by Prof. Kimberly A. Prather and her associates at the University of California, Riverside (Gard *et al.*), TSI Model 3800 is the first single-airborne-particle mass spectrometer available commercially. Its transportable design allows it to be moved between measurement sites with minimal setup or reconfiguration. It rolls through standard 36-inch-wide doorways. It also has a computer for data collection built inside the instrument cart.

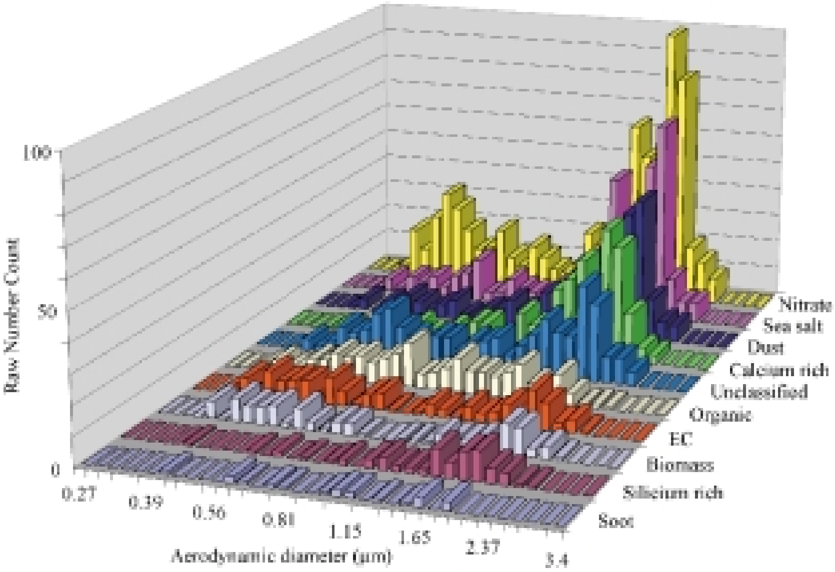
Determines size and chemical composition of single particles

The Model 3800 ATOFMS provides single particle size and composition measurements in the particle size range from 0.3 to 3 micrometers (up to 10 micrometers with optional dispersion accessory). It uses an aerodynamic sizing technique similar to that employed by our Aerodynamic Particle Sizer® and Aerosizer® spectrometers. The aerodynamic size data serves as a timing trigger and calculates when each particle will be in the focal zone of an ablation laser. This laser desorbs and ionizes the particle for chemical analysis in a bipolar, time-of-flight mass spectrometer. Mass spectral composition analysis is completed at a rate of up to 10 particles per second. Bipolar ion detection—where positive and negative mass spectra are obtained for each particle using separate ion detectors—gives you additional information about the particle and its source. Windows®-based software controls instrument functions and data acquisition.



Because the ATOFMS identifies the specific chemical compounds that make up each particle, it offers new insights into the dynamic chemistry between particles and surrounding gases, as well as other particles. Its nearly immediate composition analysis eliminates problems associated with traditional aerosol sampling onto a filter or impactor plate, such as possible secondary chemical reactions or losses of semivolatile compounds.

SOFTWARE

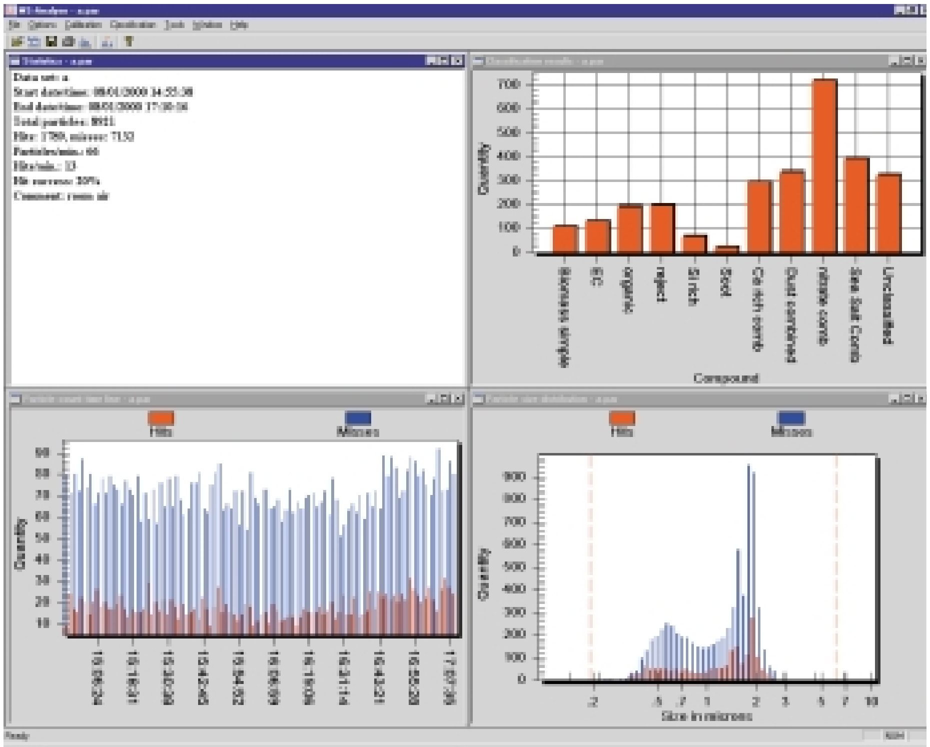


When running continuously, the ATOFMS typically generates 1 to 8 gigabytes of bipolar mass spectra and associated data per day. Therefore, effective analysis software is needed to process and store this large amount of data.

The ATOFMS uses two software packages, both of which are included with the instrument. The *MassSpec* operational software is a Windows®-based, C++ program that controls instrument operation. It also displays and saves positive and negative spectra together with the associated size. The *MS-Analyze* analytical software allows for analysis of the output from the MassSpec software. Particle size and related mass spectral data may be displayed through tables, graphs, and statistical lists.

MS-Analyze is based on a Microsoft® Access database, which allows for powerful searches in the acquired dataset. Particles may be classified based on the presence, absence, or intensity of specific peaks. The search may be limited to include only particles of a specific size range or sampling period, or within a certain ordinal count range.

As size, mass spectra, and time of detection are recorded for each individual particle, size histograms for a whole dataset, for specific time windows, or for certain types of particles can be calculated. If classes are selected so that each particle can only belong to a single class (known as *exclusive classification*), pie charts displaying percentage composition of the whole sample can be generated from the data. Average spectra of selected classes, size ranges, or times may be calculated, as well.



Data set: a
Start date/time: 08/01/2000 14:55:38
End date/time: 08/01/2000 17:10:16
Total particles: 8921
Hits: 1789, misses: 7132
Particles/min.: 66
Hits/min.: 13
Hit success: 20%
Comment: room air

A 3-D histogram of an ATOFMS classification result is shown above. The computer screen at left shows an MS-Analyze workspace displaying windows with statistical data, classification results, hits and misses by the desorption/ionization laser over time, and a size distribution of hits and misses.

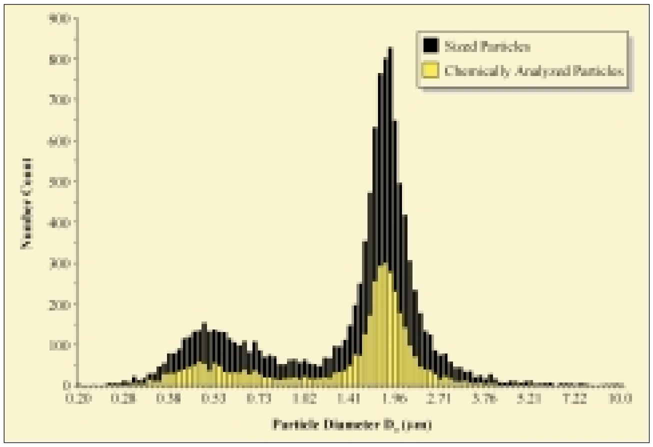
COMPOUND ANALYSIS

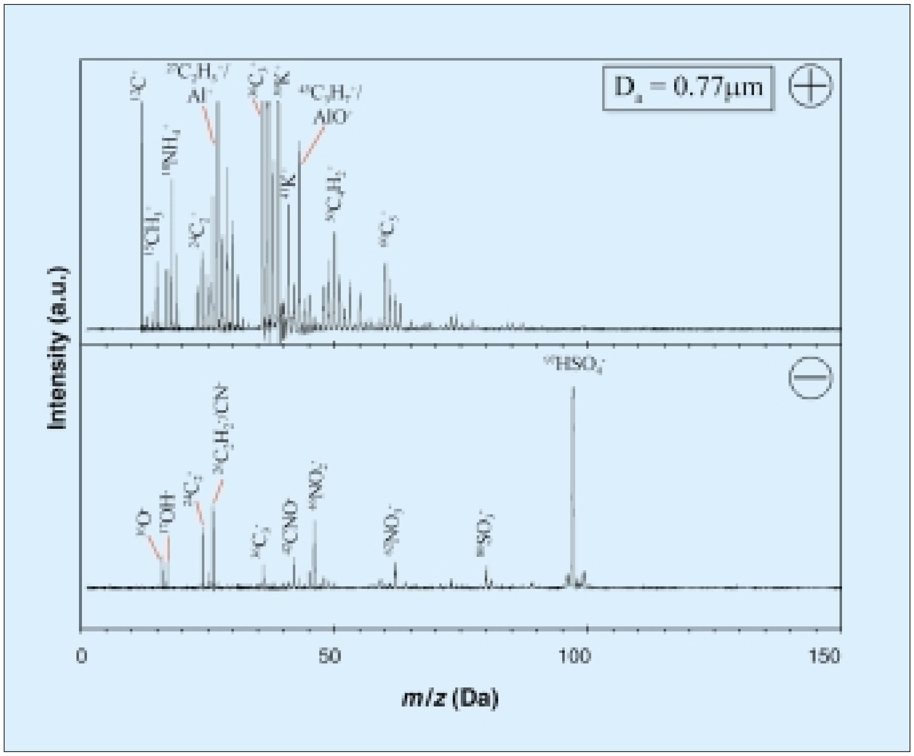
Fragments of inorganic compounds formed during the ionization process are commonly made up of single elements and molecular ions, as well as cluster ions in an oxygen-rich atmosphere, containing one or two elements and oxygen. In particles containing transition metals, the oxide is typically present, too. The detection limit for sodium ions (Na^+) is 4×10^{-16} mol with higher response for heavier alkali metals. This is consistent with periodic trends in both ionization potential and lattice energy (Gross *et al.*).

Many organic compounds give positive mass spectra that are similar to those found in libraries of 70-eV electron impact (EI) mass spectrometry (Silva and Prather). In comparison, protonated ions are expected from compounds containing polar functional groups. Negative mass spectra of organic compounds largely show carbon cluster fragments and contain fragments indicating the presence of electronegative ions such as oxygen and nitrogen.

The many *polyaromatic hydrocarbons* (PAHs) have a large absorption cross-section because 266-nanometer light induces a resonant process, which leads to high sensitivity when compared to other organic compounds. The detection limit for PAHs is on the order of 10^{-18} mol (Morrical *et al.*).

Extensive fragmentation may make it hard to distinguish between compounds in a particle containing many organics. However, it is often possible to determine specific classes of particles (PAHs, aliphatics, organic acids, etcetera) based on a fingerprint or combination of peaks. The dual-polarity ion-analysis capabilities of the ATOFMS enhance the identification of several specific classes of compounds such as organic acids and salts.





The histogram above shows the qualitative particle size distribution of an ambient aerosol sample as measured by the ATOFMS (with no correction for particle losses). Detected particles appear in black; chemically analyzed particles in yellow. This data was taken in Shoreview, Minnesota, USA on May 8, 2001, between 13:41:24 and 16:26:54. The mass spectra at left show the analysis of a single ambient organic particle taken from the same aerosol sample. Positive ions are displayed on top; negative ions on the bottom. The presence of peaks due to hydrocarbon clusters and potassium (m/z = 39 and 41) suggests that this particle was created by biomass burning. This is further supported by peaks in the negative spectrum at m/z = 26 (CN^-), 42 (CNO^-), 80 (SO_3^-), and 97 (HSO_4^-) (Silva et al.*).*

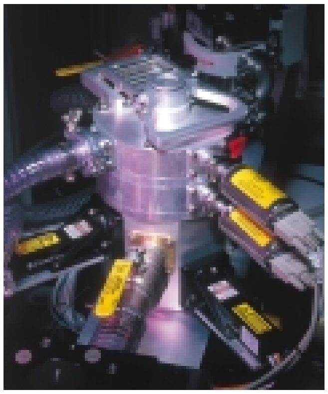
APPLICATIONS

The Model 3800 is the first commercial instrument to determine particle size and chemical composition in near real time. Applications include:

- Analytical aerosol research
- Atmospheric particle characterization, such as emission source identification
- Semiconductor processing
- Hard-disc-drive crash tests
- Indoor-air-quality monitoring
- Aerosolized-drug-delivery research
- Inhalation toxicology studies
- Drug-enforcement sample analysis
- Chemical and biological aerosol detection
- Engine emission measurements
- Powder manufacturing quality and process control for pigments, ceramics, polymers, pharmaceuticals, toners, and food powders

OPERATION

The Model 3800 ATOFMS employs two distinct time-of-flight technologies. One determines particle size; the other determines particle chemical composition. Gas-borne particles enter the ATOFMS inlet nozzle at atmospheric pressure (760 Torr)*. The pressure drops to 2 Torr at the nozzle exit. This drop in pressure causes a supersonic expansion of the gas that contains the aerosol particles. Due to their lower inertia, small particles accelerate more rapidly than large particles and obtain a higher



The interior view of the Model 3800 ATOFMS above shows the aerosol inlet, the particle sampling region, and the particle sizing region with its dual sizing lasers.

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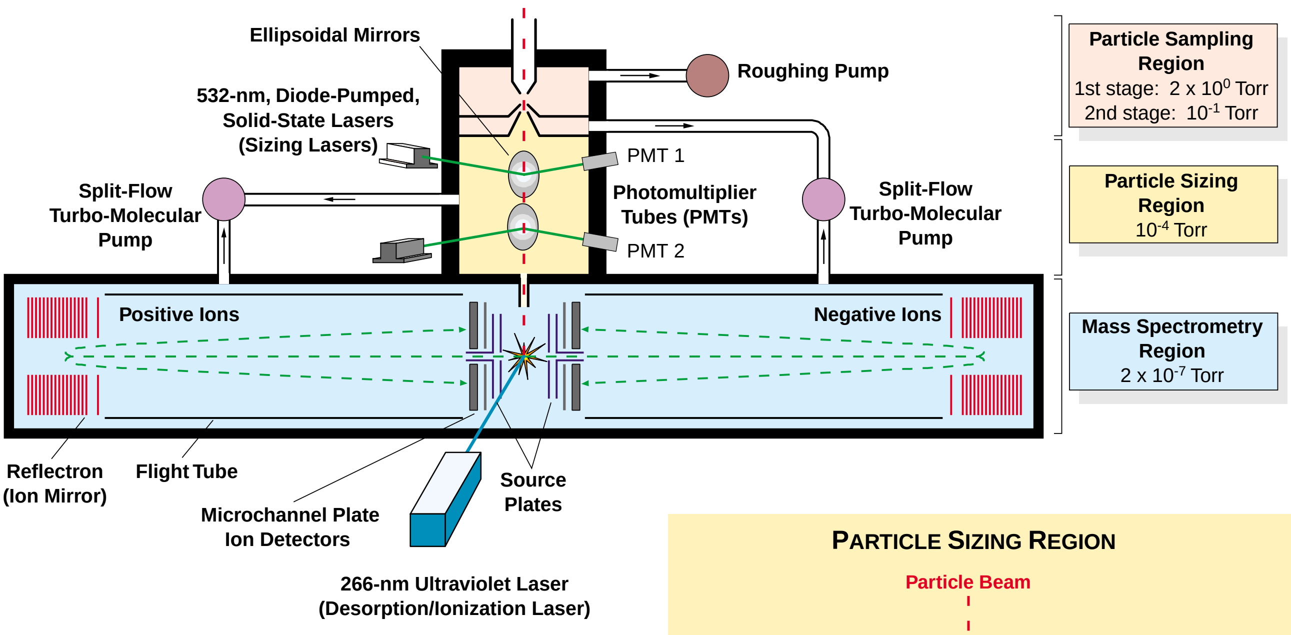
*Pressure values discussed in this document are nominal.

MODEL 3800 FLOW SCHEMATIC



terminal velocity during the expansion. After exiting the nozzle, the aerosol passes through two stages of differential pumping. This reduces the pressure to 10^{-4} Torr by the time the aerosol leaves the *particle sampling region*.

Once inside the *particle sizing region*, particles pass through a green, continuous-wave, diode-pumped solid-state (DPSS) laser, which generates an initial pulse of scattered light. A second DPSS laser, oriented orthogonally to the first, generates a second scatter pulse. The pulses are detected by two photomultiplier tubes (PMTs), one for each laser. The instrument determines particle velocity by measuring each particle's transit time between the two laser beams. This transit time is then translated into particle diameter based on an internally stored size calibration.

Next, the particles enter the *mass spectrometry region*, which is kept at a pressure of 2×10^{-7} Torr. The particle velocity measured in the particle sizing region is used to predict that particle's arrival at the ion source. A pulsed, ultraviolet laser fires, desorbing and ionizing the particle. The resulting ions are accelerated by positive and negative electric fields created by a series of source plates at different voltages. Ions with a lower mass-to-charge ratio (m/z) are accelerated to higher velocities than ions with a higher ratio. The ATOFMS contains separate flight tubes for positive ions and negative ions. It measures the time-of-flight of both ion types as they travel from the ion source to their respective ion detector.

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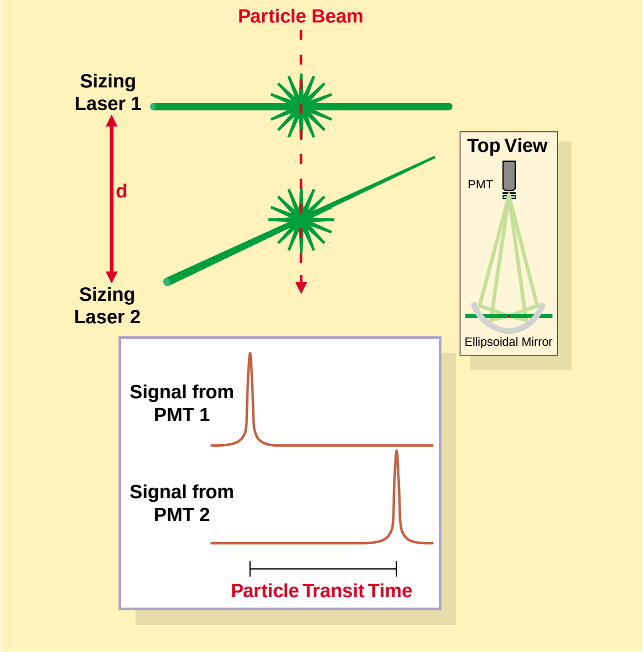
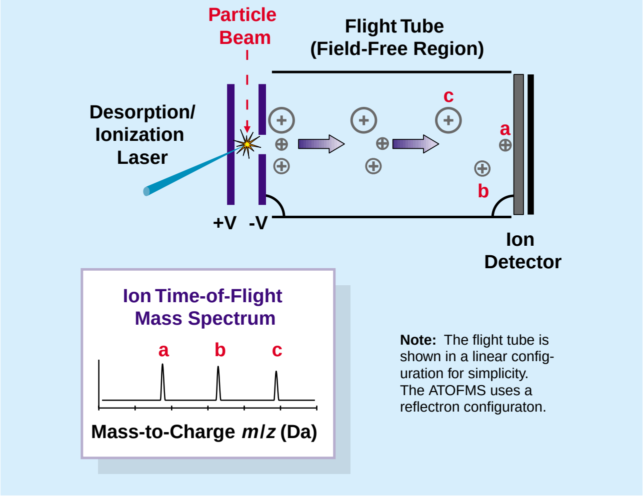
PARTICLE SIZING REGION



MASS SPECTROMETRY REGION



Note: The flight tube is shown in a linear configuration for simplicity. The ATOFMS uses a reflectron configuraton.

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Reflectrons improve the spectral resolution of the instrument by compensating for any spread in the kinetic energy of the ions. Ions of the same *m/z* can have different kinetic energies due to different initial acceleration rates during the desorption and ionization process. High-energy ions travel faster than those of lower energy, but they stay in the reflectron for a longer period of time. As a result, ions of the same *m/z* arrive at the detector with less spread, which means improved mass spectral resolution. As a secondary benefit, the flightpath length is doubled (increasing the mass spectral resolution even further) without having to increase the length of the flight tubes, and therefore, the length of the instrument.

SPECIFICATIONS

Particle size range: 0.3 to 3 µm high-resolution sizing, 0.3 to 10 µm with optional dispersion accessory†
Particle type: Airborne solids and nonvolatile liquids
Display resolution: 32 channels per decade of particle size (logarithmic), 34 channels total
Mass range‡: 1 to 800 Da
Resolution of mass spectra‡: 500 m/Δm
Total inlet flow rate (volumetric): 0.9 ± 0.05 L/min
Operating temperature: 10 to 35 °C (50 to 95 °F)
Storage temperature: 5 to 50 °C (40 to 120 °F)
Operating humidity: 0 to 75% RH, noncondensing
Maximum operating altitude: 2000 m (6562 ft)
Laser sources
Particle-sizing lasers: 50 mW at 532 nm
Desorption/ionization laser: 5 mJ/pulse at 266 nm, maximum pulse rate of 20 Hz
Detectors
Particle size: Two photomultiplier tubes (PMTs)
Ion: Two microchannel plates (MCPs)
Dimensions (LWH): 170 cm × 74 cm × 130 cm (67 in. × 29 in. × 51 in.)
Weight: 360 kg (790 lbs)
Power: 220 to 240 VAC, 50/60 Hz, 4 kW maximum

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TO ORDER

Aerosol Time-of-Flight Mass Spectrometer

Specify	*Description*
3800	ATOFMS instrument and software

Accessory

Specify	*Description*
3306	Impactor Inlet (extends size range to 10 µm)

†Transmission efficiencies are dependent upon size.
‡Mass range and resolution are dependent upon instrument conditions and settings.

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P/N 1933798 Rev. B *Published in U.S.A. (080201)*