

## INDIAN INSTITUTE OF TECHNOLOGY BOMBAY MATERIALS MANAGEMENT DIVISION Powai, Mumbai 400076.

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## Gas Chromatograph Mass Spectrometer (GCMS) System – (Qty-1 No.) Technical Specifications

Gas Chromatograph with Mass Spectrometer for analysis of CH4, CO2 (with specific 13CO2 isomer) and other compounds in reactor gas and liquid samples. The GCMS should have the following minimum configuration:

- 1. GC Mainframe
- 2. Column Oven
- 3. Split/Splitless Injector
- 4. Quadrupole MS
- 5. Autosampler
- 6. Gas Sampling Valve (GSV)
- 7. Data Management and Acquisition System
- 8. Software System
- 9. Database/Library
- 10. Columns, Spares and consumables
- 11. Training
- 12. Others

Sr.	Item Description	Detailed Technical Specification	Technical	Additional
No			_	Information
			(Yes / No)	(if any)
1.	GC Mainframe	a. Should support 3 inlets, 4 detectors and 4		
		signals acquisition.		
		b. Must be able to install up to 6 electronic		
		flow control units, providing control of up		
		to 16 or more channels.		
		c. Must have advanced intelligent self-		
		diagnosis feature. Electrical system, flow		
		control systems and sensors must be fully		
		supported by the operating software.		
		d. Must provide software that monitors GC		
		counters and provides graphic display.		
		Also must provide a real-time notification		
		via indicator/advisor when a counter limit		
		has been reached for consumables such		
		as injector port septum, glass insert (liner) and coolant.		
		e. GC must have a full colour touch screen		
		display with Graphical User Interface		
		(GUI).		
		f. One button access to service,		
		maintenance and log from the keyboard		
		must be available.		
		g. Pre-programmed leak tests must be		
		available from keyboard or monitor		
		software for safety purposes.		
		h. Standard atmospheric pressure and		
		temperature compensation must be		
		available.		
		i. Upgradability for Heart Cut GC System,		
		Detector Splitting System (multiple		
		detection capability), Detector Switching		
		System, and/or Back flush System with		

		easy-to-use dedicated integrated Advanced Flow Technology Software.  j. Retention time repeatability: <0.008% (or equivalent to 0.0008min)  k. Area repeatability: <0.5% RSD  l. Should have self-diagnosis function with safety features which helps prevent unexpected instrument malfunctions and enables a detailed diagnosis of the septum and insert usage status, whether there is a temperature sensor error, gas supply pressures, control status of each gas, ignition function, DC voltage, AD converter, and other factors.  m. Must be an Eco-GC with Gas Saver function that considerably reduces carrier gas consumption after injection or on stand-by.  n. Must have auto-shutdown feature that configures the GC to shutdown automatically after a batch run to conserve energy and gas  o. Must support Both LAN and USB communications.
2.	Column Oven	<ul> <li>a. Operating temperature range: ambient + 2°C to 450°C</li> <li>b. Oven temperature set point resolution must be 0.1°C.</li> <li>c. Oven must support at least 32 ramps and negative ramps must be allowed.</li> <li>d. Maximum achievable temperature ramp rate must be 120°C/min.</li> <li>e. Oven temperature program set point resolution for the temperature ramp rate must be 0.1°C.</li> <li>f. Maximum run time of at least 9999.99%</li> <li>g. Oven cools down from 450°C to 50°C must be in 3.4 mins, with built-in programmable oven cool-down rate</li> </ul>

		available to cater for columns of different stability.	
		h. Built-in oven light that facilitates column installation.	
3.	Split/Splitless Injector	a. Must be able to install at least 2 independent temperature controlled injector unit	
		b. Must be suitable for all capillary columns of 50um to 530um internal diameter.	
		c. The pressure controller must come with compensation for barometric pressure and ambient temperature changes as standard.	
		d. Must be able to select pressure units as psi, kPa or bar.	
		e. Must be able to select carrier and makeup gas types: Helium, Hydrogen, Nitrogen or Argon.	
		f. Split ratio range: 0 to 9999 must be available to avoid column overload.  Maximum operating temperature at least 450°C or more.	
		g. Must consist of at least 3 pressure programming methods, including the constant linear velocity mode.	
		h. Number of pressure programming steps must be at least 7 or more.	
		i. Pressure setting range: 0 to 1035 kPa (0 to 150 psi)	
		j. Pressure sensor should be accurate up to 2% at full scale, with repeatability within 0.34kPa (or 0.05psi).	
		k. The pressure has to be stable against temperature coefficient within 0.68kPa/oC (or 0.1psi/oC) change, and	
		has a drift of less than 0.68kPa/6mth (or 0.1psi/6mth).  I. Number of flow programming steps must	
		be at least 7, with higher number preferred.	

		m. Flow sensor should be accurate up to 5% of set point, with repeatability within 0.35% of the set point.  n. The flow has to be stable against temperature coefficient within 0.2%/oC change.  o. Must be able to set total flow range: 0 to 1,300mL/min for He, 0 to 1,300mL/min for H2, 0 to 600mL/min for N2.  p. Built-in automatic carrier shutoff if the inlet pressure drops significantly, i.e. in the case of leakage.  q. Efficient gas saver mode built-in to reduce gas consumption during standby without affecting performance.  r. Must have electronic septum purge flow control to eliminate carry-over.	
4.	Quadrupole MS	<ul> <li>a. The quadrupoles should be made up of metal rods and must be easily cleanable.</li> <li>b. The quadrupoles must have the pre-rods as filter to minimize the influence of contamination and thus increase the sensitivity.</li> <li>c. The mass spectrometer must have Electron Ionization (EI) modes supplied as standard. Positive Chemical Ionization (PCI) and Negative Chemical Ionization (NCI) modes should be available</li> <li>d. The mass spectrometer must be equipped with an ultra-high sensitivity ion source that has an ion optical system with high transport efficiency and excellent temperature homogenization of the ion source box to prevent the formation of adsorption sites inside the ion source due to cold spots.</li> <li>e. Should have a mass range of 1.5 to 1090 amu with unit mass resolution over the entire mass range.</li> </ul>	

- f. Should provide one click auto-tune for BFB, DFTPP.
- g. Should be able to perform calibration manually as well as auto-tune at m/z 1066 [Tris(perfluorononyl)-S-triazine), molecular weight of 1485] to obtain accurate mass spectrum for high molecular weight compounds such as halogenated and derivatized compounds.
- h. The mass spectrometer should be able to scan at faster scan rate in order to achieve more information and more data points for accurate quantitation. The scanning speed capability should be 20,000 amu/sec (single scan). Higher scan rates are preferred
- i. Should have faster scan cycles in order to obtain highly precise data for fast GCMS and should be able to support advance applications such as comprehensive GC x GC.
- j. The mass spectrometer should have a stability of +0.1u / 48 hours.
- k. The ion source and transfer line must be independently heated over a user-selectable temperature range:
  - i) Ion Source: 100 to 350°C
  - ii) Transfer Line: 50 to 350°C
- I. The ion source must be accessible from the front for ease of maintenance without the need to remove the top cover.
- m. The mass spectrometer should have Twin-Line capability to eliminate the need to swap columns when switching applications.
- n. The mass spectrometer must have a dynamic range of 8 x 106.
- Should have high performance synchronous SIM/Scan with automated SIM set up that can convert a full scan method to a SIM or SIM/Scan method.

- The software must automatically configure the number of SIM group, SIM cycles across the peak and the ions added to each group.
- p. Software must have automatic SIM table creation function included to create SIM window base on elution time.
- q. Should be able to automatically set up a SIM/Scan method from an injected standard.
- r. Should have a SIM capability of up to 64 groups of masses with 128 masses per group may be time programmed.
- s. The mass spectrometer should employ a unique over-drive lens to minimize random noise enhancing the Signal-to-Noise.
- t. El scan sensitivity: Signal-to-noise (S/N)
   > 2000 at m/z 272 for 1 pg
   Octafluoronapthalene (OFN) in El scan
- u. The vacuum system should consist of high capacity turbo molecular pump with differential vacuum exhaust system. Minimum 300 L/Sec capacity is required higher capacity is preferred to allow higher flow rates at least 8 ml/min or more.
- v. The mass spectrometer should have capability to install two narrow-bore capillary columns into the MS simultaneously to eliminate the need to swap columns.
- w. There should be an automatic interrupt system which provides protection against damage such as filament failure. In case of power failure, vacuum integrity and cleanliness should be maintained by not venting to atmospheric pressure automatically.

		<ul> <li>x. There should be 2 filaments available for EI ionization mode allowing automatic switching to another when one fails.</li> <li>y. Fully automatic start-up and shut-down of the GCMS by simply one-click of a button on the computer screen must be available when replacing columns or repairing ion sources.</li> <li>z. Should have eco-friendly feature which reduces the power consumption in analysis standby mode.</li> </ul>
5.	Autosampler	<ul> <li>a. Sample injection system should accommodate at least 12 sample vials.</li> <li>b. Must allow random access in sample sequencing.</li> <li>c. Must have priority sampling mode to allow priority sample and method to be inserted into the sequence at any time.</li> <li>d. Number of sample injections: 1 ~ 99 injections per sample.</li> <li>e. Sample volume injection should be in the range of 0.1 ~ 8.0 μl. Optionally, should be capable of 0.5 ~ 40 μl &amp; 2.5 ~ 200 μl injection.</li> <li>f. Syringe speed: Selectable in two stages.</li> <li>g. Plunger movement speed: Selectable in three stages.</li> <li>h. Cross contamination of &lt;10-4.</li> <li>i. Number of syringe pumping: 0 ~ 20 with pre-wash and post-wash after injection of samples.</li> <li>j. Depth of syringe insertion into the vial: Changeable in up-down directions to access different layer of sample solution.</li> <li>k. Solvent flush method and Standard Addition Mode should be available.</li> <li>l. Multi-injection up to 18mL should be possible for large volume injection.</li> <li>m. Area repeatability of injection amount must be less than 2%.</li> </ul>

		n. Able to prepare ahead, for example washing the syringe with solvent prior to the next analysis.
6.	Gas sampling valve (GSV)	<ul> <li>a. System should be provided with suitable automatic Gas sampling valves, suitable loops, separate temperature control valve box (up to 150°C or more), columns and related accessories for automatic gas sampling &amp; injecting to column to get desired analysis.</li> <li>b. Valve should be housed in separate box on the top of GCMS unit.</li> <li>c. Pressure balance or Sample start/stop valve should be included to automatically stop the sample flow from cylinder once the sample is done and it should start the sample flow automatically when GC is ready for next sample injection.</li> </ul>
7.	Data Management and Acquisition System	a. Data Management b. Intel i5 processor or better c. 16GB RAM Memory d. 500GB Hard disk Storage e. 21" LCD monitor f. 101 keys keyboard g. Mouse & mousepad h. Windows 11 Pro licensed version i. MS Office latest version j. Antivirus software
8.	Software System	<ul> <li>a. The system should be an easy-to-use next generation 32-bit software that incorporates the latest Windows technology.</li> <li>b. Equipped with multiple functions like Graphical User Interface, Assistant Bar, Data Explorer, Wizard software and long-filename compatible.</li> <li>c. Flexible Graphical User Interface to display instrument status, show real time plot and change all instrument set points.</li> </ul>

- d. Able to identify target analyte correctly in the event where retention time has shifted from the originally supposed retention time.
- e. The software package should allow for the complete control of the GC. Furthermore, the software must include the capability to control up to 4 GCs at any one time (9 detectors simultaneously), method development and automation, data acquisition, data analysis, generation of custom reports, etc.
- f. Should have full GLP/GMP support in terms of security, audit-trail and validation support.
- g. Must have the following data acquisition capabilities:
  - i. Snapshot function, supports single analysis and batch analysis, Batch Table Wizard, add or insert analyses.
  - ii. Supports extended analysis time, automatic time, automatic data file creation.
  - iii. QA/QC (statistical) functions, batch auto-stop function, run user program function, supports prerun programs, OLE automation compatibility (Batch analysis, etc).
- h. Must have the following data processing and data analyses functions:
  - i. Peak integration manipulation, identification (supports multiple relative retention times and grouping)
  - ii. Quantitation (percentage area method, corrected percentage area method, internal standard method, external standard method, standard addition

		method, index calculation, manual coefficient input)  iii. Calibration points and levels (16 levels x 10 points), manual calibration curve creation, column performance calibration, data comparison functions.  i. Must have more than 10 types of report items – sample information, environment settings, methods, chromatograms, peak tables, calibration curves, grouping results, diagrams, text, etc.), OLE object compatibility, layout customization and preview functions, summary report.  j. Must allow clock-time programming with the ability to automatically start/stop a GC at the user-specified scheduled time.  k. Must be capable of performing detector auto-ranging.  l. System check (GC self-diagnosis), status log must be available to allow continuous monitoring of GC in real-time to alert user maintenance needs and instrument problems.
9.	Library	a. NIST 2023 Mass Spectral library or latest should be included.
10.	Columns, Spares and consumables that must be included with the system	<ul> <li>a. GCMS startup kit with suitable capillary column for MS tuning and installation checkout criteria and capillary columns as per application.</li> <li>b. Set of GCMs consumables kit which includes – Injector Septum, Split inserts, Splitless inserts, Graphite ferrules for all column sizes (10nos each), Vespel ferrules for all column sizes (10nos each), Quartz wool, column nuts (15nos), Orings, Capillary adapter, nipple for gasket. Approx qty for usage up to 1.5 to 2 years of operation.</li> </ul>

		<ul> <li>c. One box of 100 samples vials with caps suitable for GC injection</li> <li>d. Set of Maintenance kit which Includes split filter for flow/ pressure controller -1 pc; filament - 2 pcs; Ion source polisher – 1no; gold packing- 1 pc; aluminum packing - 100 pcs; insulator bush- 1 pc.</li> </ul>
11.	Training	<ul> <li>a. The supplier must provide training for the users of the instruments at site as well as at the supplier's application laboratory, after installation and commissioning. Details of the training program must be attached with the tender.</li> <li>b. Training should be provided for all the respective department users.</li> </ul>
12.	Others	<ul> <li>a. The supplier must demonstrate that it has a proven appropriate set-up and capability to provide after-sales service efficiently and effectively. The supplier should have in his facility a similar system to that proposed in this tender for training purpose.</li> <li>b. Software upgrades like version ups, if any, should be done without any additional cost.</li> <li>c. All modules must be GLP compliant.</li> <li>d. A declaration of Conformity certificate must be provided.</li> <li>e. A declaration of System Validation certificate must be provided.</li> </ul>
13.	Service, Warranty and Training	<ul> <li>a. The system should be accompanied with Conformity Certificate.</li> <li>b. Tendered price should include delivery, installation, commissioning and training (at least 3 users) at customer's location.</li> <li>c. On-site installation, commissioning and training should be conducted by a qualified factory trained engineer.</li> </ul>

- d. Complete support with instrument warranty for equipment for at least a period of 24 months. This shall include the following at no extra cost
  - i. Travel and Labour expenses of Customer Engineer.
  - ii. Service Parts used for repairs.
- e. The vendor shall provide a comprehensive service guarantee during the warranty period. In the event that the system requires service, the vendor shall repair or replace the instrument at no additional cost.
- f. Vendor to have logistic support to ensure that over at least 95% of the service parts are readily available and upkeep delivery within 24 hours.
- g. The warranty shall commence only upon successful completion of the Acceptance Test, Commissioning and Training.
- h. Support should be available from Monday to Friday, 8.30am to 5.30pm (excluding Public Holidays)
- i. Vendor to provide a copy of Site-Preparation checklist.
- j. Vendor to provide both on-site and operator training for users on the system start-up, usage, maintenance, quality control, trouble shooting, etc. including comprehensive classroom training.