

SEMI C3.39-1011 (Reapproved 0118) SPECIFICATION FOR NITROGEN TRIFLUORIDE (NF₃), 99.98% QUALITY

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1 Purpose

1.1 The purpose of this Document is to provide specification for nitrogen trifluoride (NF₃) that is used in the semiconductor industry.

2 Scope

2.1 This Document covers requirements for nitrogen trifluoride (NF₃) used in the semiconductor industry.

NOTICE: SEMI Standards and Safety Guidelines do not purport to address all safety issues associated with their use. It is the responsibility of the users of the Documents to establish appropriate safety and health practices, and determine the applicability of regulatory or other limitations prior to use.

3 Referenced Standards and Documents

3.1 None.

4 Description

4.1 Nitrogen trifluoride is a toxic, odorless, colorless, nonflammable gas. It is a strong oxidizer and supports combustion.

5 Specifications

Table 1 Impurity Limits for Nitrogen Trifluoride

Grade	99.98%
Impurities	Maximum Acceptable Level (ppm) ^{#1}
Carbon Dioxide (CO ₂)	10
Carbon Monoxide (CO)	10
Carbon Tetrafluoride (CF ₄)	100
Nitrogen (N ₂)	10
Nitrous Oxide (N ₂ O)	10
Argon/Oxygen	10
Sulfur Hexafluoride (SF ₆)	10
Water (H ₂ O) (v/v)	1
TOTAL IMPURITIES	161 ^{#1}

#1 An analysis of significant figures has not been considered. The number of significant figures will be based on analytical accuracy and the precision of the provided procedure.

6 Chemical Specification

6.1 Hydrolyzable Fluorides as HF: 1 ppm.

7 Properties of Nitrogen Trifluoride (for information only)

Table 2 Properties of Nitrogen Trifluoride

	<i>Metric Units</i>	<i>US Units</i>
Molecular Formula	NF ₃	NF ₃
CAS Number	7783-54-2	7783-54-2
Molecular weight	71.00	71.00
Density of gas at 21.1°C (70°F) and 101.3 kPa (1 atm)	2.94 kg/m ³	0.1838 lb./ft. ³

8 Analytical Procedures

8.1 *Carbon Tetrafluoride* — This procedure is for the determination of carbon tetrafluoride in nitrogen trifluoride using a gas chromatograph with a thermal conductivity detector (see Figure 1).

NOTE 1: Pass the carrier gas through a trap (3 m [10 ft.] by 6.4 mm [¼ in.] OD) containing 50% by volume molecular sieve 5A and 50% by volume molecular sieve 13X submerged in liquid nitrogen.

8.1.1 *Detection Limit* — 1.0 ppm.

8.1.2 *Instrument Parameters*

8.1.2.1 Column: Super Q (80/100 mesh), 4.9 m (16 ft.) by 1.75 mm (1/16 in.) ID, 3.2 mm (1/8 in.) OD ss or equivalent.

8.1.2.2 Carrier Flow: 19 mL/min helium.

8.1.2.3 Sample Volume: 0.1 mL.

8.1.2.4 Temperatures:

- Detector: 100°C.
- Oven: 42°C.
- Gas sampling valve: 42°C.

8.1.2.5 Valve material: Nitronic-60 or equivalent.

8.1.3 *Calibration Standard* — 100 ppm carbon tetrafluoride, balance helium.

8.1.4 *Operating Procedure*

8.1.4.1 Inject the calibration standard into the column using a gas sampling valve. Record retention time and peak area.

8.1.4.2 Inject nitrogen trifluoride sample to be tested in the same manner as the calibration standard. Record the retention times and peak areas.

8.1.4.3 Repeat ¶ 8.1.4.1.

8.1.4.4 Compare the average peak area of the calibration standard to that of the nitrogen trifluoride sample being tested. Calculate the concentration of carbon tetrafluoride, using the formula below. The result may not exceed the specification in § 5 of this Standard.

$$\frac{\text{Sample Peak Area}}{\text{Standard Peak Area}} \times \text{Concentration of Standard} = \text{Concentration of Sample} \quad (1)$$

8.2 *Carbon Dioxide, Nitrous Oxide, and Sulfur Hexafluoride* — This procedure is for the determination of carbon dioxide, nitrous oxide, and sulfur hexafluoride in nitrogen trifluoride using a gas chromatograph with a thermal conductivity detector (see Figure 1).

8.2.1 *Detection Limit* — 1.0 ppm for carbon dioxide, nitrous oxide, and sulfur hexafluoride.

8.2.2 Instrument Parameters

8.2.2.1 Column: Super Q (80/100 mesh), 4.9 m (16 ft.) by 1.75 mm (1/16 in.) ID, 3.2 mm (1/8 in.) OD ss or equivalent.

8.2.2.2 Carrier Flow: 19 mL/min helium.

8.2.2.3 Sample Volume: 1.0 mL.

8.2.2.4 Temperatures:

- Detector: 100°C.
- Oven: 42°C.
- Gas sampling valve: 42°C.

8.2.2.5 Valve Material: Nitronic-60 or equivalent.

8.2.3 Calibration Standard — 10 ppm carbon dioxide, 10 ppm nitrous oxide, 10 ppm sulfur hexafluoride, balance helium.

8.2.4 Operating Procedure

8.2.4.1 Inject the calibration standard into the column using a gas sampling valve. Record the retention times and peak areas. The order of elution is carbon dioxide, nitrous oxide, sulfur hexafluoride. (See Figure 1 for valve configuration.)

8.2.4.2 Inject the sample to be tested in the same manner as the calibration standard. Record the retention times and peak areas.

8.2.4.3 Repeat ¶ 8.4.2.1.

8.2.4.4 Compare the average peak area of the calibration standard to that of the nitrogen trifluoride sample being tested. Calculate the concentration of each impurity using the formula below. The results may not exceed the specifications in § 5 of this Standard.

$$\frac{\text{Sample Peak Area}}{\text{Standard Peak Area}} \times \text{Concentration of Standard} = \text{Concentration of Sample} \quad (2)$$

8.3 Carbon Monoxide — This procedure is for the determination of carbon monoxide in nitrogen trifluoride using a gas chromatograph with a methanizer and a flame ionization detector (see Figure 1).

NOTE 2: The methanizer catalyst can be destroyed by nitrogen trifluoride passing through to at high temperature. After the carbon monoxide peak is detected, the bulk nitrogen trifluoride is bypassed to vent by means of a four-port switching valve installed downstream of the separating column and before the methanizer (see Figure 1).

8.3.1 Detection Limit — 0.1 ppm.

8.3.2 Instrument Parameters

8.3.2.1 Column: Carbosphere (80/100 mesh), 0.74 m (2.4 ft.) by 1.75 mm (1/16 in.) ID, 3.2 mm (1/8 in.) OD ss or equivalent.

8.3.2.2 Carrier Flow: 25 mL/min helium.

8.3.2.3 Sample Volume: 0.5 mL.

8.3.2.4 Fuel gases:

- Hydrogen: Zero grade or better hydrogen at a flow rate of 45 mL/min is added to the carrier gas between the column outlet and the methanizer inlet.
- Air: Zero grade or better air is used at a flow rate of 300 mL/min.

8.3.2.5 Temperatures

- Detector: 150°C.
- Oven: 42°C.