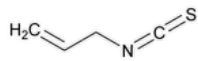


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Allyl Isothiocyanate



C₄H₅NS 99.15
3-Isothiocyanato-1-propene;
Isothiocyanic acid allyl ester CAS RN®: 57-06-7; UNII: BN34FX42G3.

DEFINITION
Allyl Isothiocyanate contains NLT 93.0% and NMT 105.0% of allyl isothiocyanate (C₄H₅NS).

[**CAUTION**—Allyl Isothiocyanate is a potent lachrymator, with a pungent, irritating odor. Care should be taken to protect the eyes, to prevent inhalation of fumes, and to avoid tasting.]

IDENTIFICATION

Change to read:

• **A.** ▲ [SPECTROSCOPIC IDENTIFICATION TESTS \(197\)](#), [Infrared Spectroscopy: 197F](#) ▲ (CN 1-MAY-2020) : The spectrum exhibits pronounced peaks at about 700, 950, 980, 1300, 1340, 1350, 1410, 1420, 1650, 2100, and 2200 cm⁻¹.

ASSAY

• **PROCEDURE**

Sample solution: Transfer 4 mL into a 100-mL volumetric flask, and dilute with alcohol to volume.
Analysis: Transfer 5.0 mL of the *Sample solution* to a 100-mL conical flask, and add 50.0 mL of 0.1 N silver nitrate VS and 5 mL of ammonia TS. Connect the flask to a reflux condenser, heat on a water bath for 1 h, and allow to cool to room temperature. Disconnect the flask from the condenser, transfer the contents of the conical flask to a 100-mL volumetric flask with the aid of water, and dilute with water to volume. Pass through a dry filter, discarding the first 10 mL of the filtrate. To 50.0 mL of the subsequent filtrate add 5 mL of nitric acid and 2 mL of ferric ammonium sulfate TS, and titrate the excess silver nitrate with 0.1 N ammonium thiocyanate VS. Perform a blank determination, using 5 mL of alcohol in place of the *Sample solution*, and make any necessary correction. Each mL of 0.1 N silver nitrate is equivalent to 4.958 mg of allyl isothiocyanate (C₄H₅NS).

Acceptance criteria: 93.0%–105.0%

IMPURITIES

• **LIMIT OF PHENOLS**

Sample solution: Dilute a 1-mL sample with 5 mL of alcohol.
Analysis: Add 1 drop of ferric chloride TS to the *Sample solution*.
Acceptance criteria: A blue color is not produced immediately.

SPECIFIC TESTS

- [SPECIFIC GRAVITY \(841\)](#): 1.013–1.020
- [REFRACTIVE INDEX \(831\)](#): 1.527–1.531, determined at 20°
- [DISTILLING RANGE, Method I\(721\)](#): 148°–154°

ADDITIONAL REQUIREMENTS

- **PACKAGING AND STORAGE:** Preserve in tight containers.

Auxiliary Information - Please [check for your question in the FAQs](#) before contacting USP.

| Topic/Question | Contact | Expert Committee |
|----------------------|---|---------------------------|
| ALLYL ISOTHIOCYANATE | Documentary Standards Support | SM32020 Small Molecules 3 |

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