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VAPOR-PHASE INFRARED ABSORPTIVITY COEFFICIENT OF HN1

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14. ABSTRACT We report the vapor-phase IR absorptivity coefficient of the vesicant chemical agent, HN1. The data are provided at a spectral resolution of 0.25 cm^{-1} (data spacing of 0.125 cm^{-1}). We describe the methods used to generate the spectra, process the raw data, and provide a comparison to ellipsometry measurements of the linear absorptivity coefficient of the compound.					
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PREFACE

The work described in this report was performed under the direction of the Detection Capability Officer, Defense Threat Reduction Agency Joint Science and Technology Office (DTRA-JSTO). This work was started in April 2011 and completed in May 2011.

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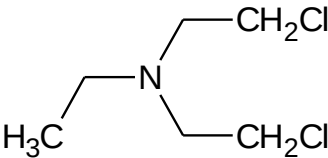
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VAPOR-PHASE INFRARED ABSORPTIVITY COEFFICIENT OF HN1

1. INTRODUCTION

The nitrogen mustards (HN1, HN2, and HN3) are similar to sulfur mustard (HD) in their physical properties and physiological effects. All are delayed-casualty agents that produce conjunctivitis, laryngitis, bronchitis, hoarseness, coughing, elevated temperature, nausea, and vomiting on exposure.¹ Selected properties of the HN1 (Table 1) were obtained from *Potential Military Chemical/Biological Agents and Compounds*, FM 3-11.9,¹ with the exception of the vapor pressure. The vapor pressure of HN1 was recomputed with updated Antoine constants from new measurements that were obtained incidental to the acquisition of the absorptivity coefficient and reported by Williams et al.²

Table 1. Selected Properties of HN1

Structural Formula	Properties
	<i>Bis</i> -(2-chloroethyl)ethylamine CAS RN: 538-07-8 Symbol: HN1 Formula: C ₆ H ₁₃ Cl ₂ N Formula weight: 170.08 Density: 1.09 g/cm ³ at 25 °C Purity: >99% <i>P</i> _{25°C} : 0.241 Torr (32.2 Pa)

Note: Values obtained from FM 3-11.9.¹

CAS RN: Chemical Abstracts Service Registry Number

2. EXPERIMENTAL SECTION

2.1 Instrument and Equipment Parameters

The system used to generate the continuous vapor stream was an adaptation of the saturator cell method developed at the U.S. Army Edgewood Chemical Biological Center (ECBC) for measuring the volatility of chemical warfare agent-related compounds.³

The method, which was modified to generate continuous streams of chemical compounds for obtaining quantitative vapor-phase IR spectra, has been used to measure the absorptivity coefficients of benzene³ as well as a variety of chemical warfare agent-related compounds.⁴⁻⁸ Tevault et al.³ describe the experimental setup, data collection, and post-processing in more detail. The saturator passed a stream of nitrogen carrier gas, which was obtained from the boil-off of a bulk liquid nitrogen tank, across an alumina Soxhlet thimble in a glass holder filled with the analyte. A vapor-liquid equilibrium of the analyte on the downstream side of the saturator cell resulted, and the concentration of the analyte was determined by the temperature of the liquid phase. When the saturator cell is suspended in a constant temperature bath, the concentration of the analyte can be predicted by its vapor pressure

at the temperature of the bath. The ECBC quantitative Fourier transform infrared spectrometer (FTIR) laboratory used a Brooks (Brooks Instrument Co., Hatfield, PA) model 5850S mass flow controller to maintain a constant flow to the saturator cell, along with a second mass flow controller to add diluent to the stream and to provide an additional means of adjusting the concentration of the compound delivered to the “White” cell (multipass gas cell) of the FTIR. Linearity of the S-series mass flow controllers are adjusted using a second-order polynomial, which results in uncertainties of approximately 1% or better for rates at flows $\geq 25\%$ of full scale.

Spectra were obtained with a Bruker (Bruker Optics, Billerica, MA) model IFS/66V FTIR spectrometer. The instrument is equipped with deuterated triglycine sulfide and mercury–cadmium–telluride (HgCdTe) detectors and was capable of obtaining spectra with a maximum spectral resolution of 0.1125 cm^{-1} (unapodized). The interferograms were recorded from $15,798$ to 0 cm^{-1} with a resolution of 0.125 cm^{-1} . Absorbance (log base 10) spectra were processed with boxcar apodization and were $2\times$ zero-filled to obtain a data spacing of 0.0625 cm^{-1} . The instrument was equipped with a variable-path White cell. The experimental data were obtained using path lengths of 4.057 , 5.377 , and 8.024 m . The temperature of the White cell was maintained at $23 \pm 0.1\text{ }^{\circ}\text{C}$ through the use of a thermostatically controlled chamber enclosing the spectrometer and cell. Data were acquired at a speed of 60 KHz (helium–neon [HeNe] laser, zero-crossing frequency) using the HgCdTe detector. Single-beam spectra of the chemical warfare agent were ratioed against spectra of clean, dry nitrogen. To minimize the effects of nonlinearity in the detector, the interferograms were processed using the proprietary Opus-IR nonlinearity correction function (Bruker Optics). All interferograms were archived, which enables further post-processing of the data. A list of instrument parameters is included in Table 2.

Table 2. Instrument Settings for the Bruker IFS-66/V FTIR Spectrometer

Parameter	Setting
Spectral resolution	0.1125 cm^{-1}
Zero fill	$2\times$ on interferogram
Apodization	Boxcar
Source	SiC glowbar
Beamsplitter	Germanium-coated KBr
Scanner speed	60 KHz
Aperture	2 mm
Detector	HgCdTe
Folding limits	15798 to 0 cm^{-1}
Phase resolution	2 cm^{-1}
Phase Correction	Mertz
Fourier transform limits	4000 to 550 cm^{-1}

Temperature and pressure data were recorded using National Institute of Standards and Technology-traceable digital barometers and thermometers, and all data were archived. Concentration–path length (CL) products were computed in units of micromoles per

mole-meter (parts per million-meter). A digital barometer had previously been used to measure the dynamic pressure in the White cell with gas flowing into the cell, and the ambient pressure was plotted versus the differential pressure. The resulting equation was used to correct the readings from the ambient pressure barometer to the pressure in the White cell. The CL data were corrected to 296 K and 1.0132×10^5 Pa (760 Torr) using the ideal gas law.

2.2 Feedstock

Analysis of an aliquot of the material using carbon-13 nuclear magnetic resonance (^{13}C -NMR) spectroscopy, gas chromatography (GC) with thermal conductivity detection (TCD), and GC with mass spectrometry (MS) yielded the results shown in Table 3.

Table 3. Results from Analysis of HN1 Sample
Used for Determination of Absorptivity Coefficient

Analytical Technique	Purity (%)
^{13}C -NMR	>99
GC-TCD	99.5
GC-MS	99.2

A sample purity of $99 \pm 1\%$ was used to calculate the mass rate of the HN1 from the delta mass of the saturator cell.

2.3 Data Processing

A total of 11 spectra were generated. Spectra were initially preprocessed by subjecting them to a four-point baseline correction using anchor points of 585, 1960, 2255, and 3548 cm^{-1} . The corrections were done in Matlab (MathWorks, Natick, MA) by performing first-order least-squares fits between successive pairs of anchor points, including 10 additional data points on each side of the anchor points. The resulting correction values of absorbance (A) were <0.002 in all cases. In our experience, when baseline drift is so small, there is little or no advantage in performing a higher-order baseline subtraction. Thereafter, spectral features arising from trace water vapor were removed by spectral subtraction.

After correcting to 296 K and 101,325 Pa, CL ranged from 94 to $599\text{ }\mu\text{mol}\cdot\text{mol}^{-1}\cdot\text{m}^{-1}$. Dividing the single-beam spectra of the agent by the single-beam spectra of the nitrogen resulted in transmittance spectra that were then further processed to absorbance spectra by

$$A(\tilde{\nu}) = -\log_{10}T(\tilde{\nu}) \quad (1)$$

where A is absorbance, $\tilde{\nu}$ is frequency, and T is transmittance.

Beer's law states that absorbance at a frequency is proportional to the CL product and the absorptivity coefficient

$$A(\tilde{\nu}) = \alpha(\tilde{\nu})CL \quad (2)$$

where α is the wavelength-dependent absorptivity coefficient. The absorbance spectra form a matrix with a size of $57,248 \times 11$. Rearranging eq 2 yields

$$\alpha(\tilde{\nu})CL = \frac{A(\tilde{\nu})}{CL} \quad (3)$$

Equation 3 can then be solved at each frequency using a least-squares approach. This was accomplished with code written in Matlab: `run_analyze_vapor_absorption_coeff.m`. Inputs for the program include: the confidence limits for the prediction of α and a maximum value of A to be used in the fit. Code for the program is available in Williams et al.⁴ Outputs include: (1) arrays with values of α and (2) statistical (Type-A) uncertainties (U_A , expressed as absorbance values). The latter output permits the fractional statistical (frac) uncertainty in the absorptivity coefficient to be calculated as

$$U(\tilde{\nu})_{A, \text{frac}} = \frac{U(\tilde{\nu})}{A(\tilde{\nu})_A} \quad (4)$$

3. RESULTS AND DISCUSSION

To perform an initial check of the quality of the data, Beer's law plots of two spectral lines, 2980.00 and 757.45 cm^{-1} , were calculated, and the results showed that the data appeared to be well fitted, at least for these two spectral lines. No points were found lying outside of the 95% confidence limits for a repeated set, for a repeated single x point, or for the 95% confidence limits for a Grubbs test for outliers.⁹ The Beer's law plots of those two lines are shown in Figure 1.

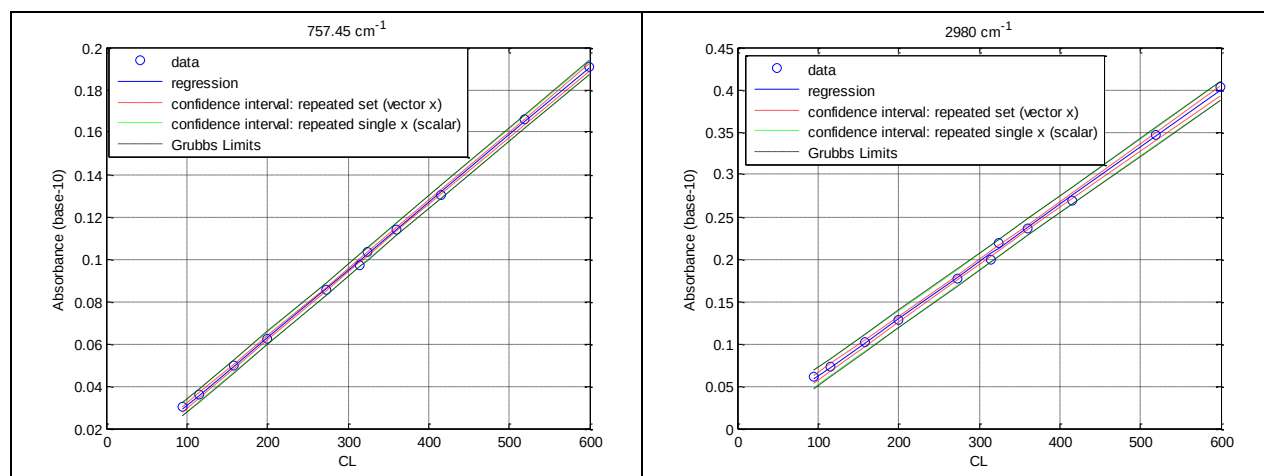


Figure 1. Beer's law plots of HN1 at frequencies of 757.45 and 2980 cm⁻¹.

The absorptivity coefficient and uncertainty (Type-A, 2σ) were then computed line by line within the spectral range of 4000 to 550 cm⁻¹. Values of $A > 1.5$ are normally assigned a weight of zero. The strongest feature in the spectrum of HN1, observed at 2979.965 cm⁻¹, has a value of $\alpha = 0.000674$, which gave only $A = 0.402$ at the highest CL. Therefore, least-squares fits of the individual spectra lines incorporated all data. Figure 2 shows the plotted absorptivity coefficient and Type-A uncertainties for the computed spectral range. The figures are plotted with α in units of (micromole/mole)⁻¹ × meter⁻¹ [(μmol/mol)⁻¹m⁻¹]. To obtain α in (milligrams/meter²)⁻¹ [(mg/m²)⁻¹], the values on the ordinate scale of Figure 4 were multiplied by 0.1420. This factor was derived by dividing the molar volume of nitrogen at the temperature of the White cell (24.15 L) by the molecular weight of HN1 (170.08).

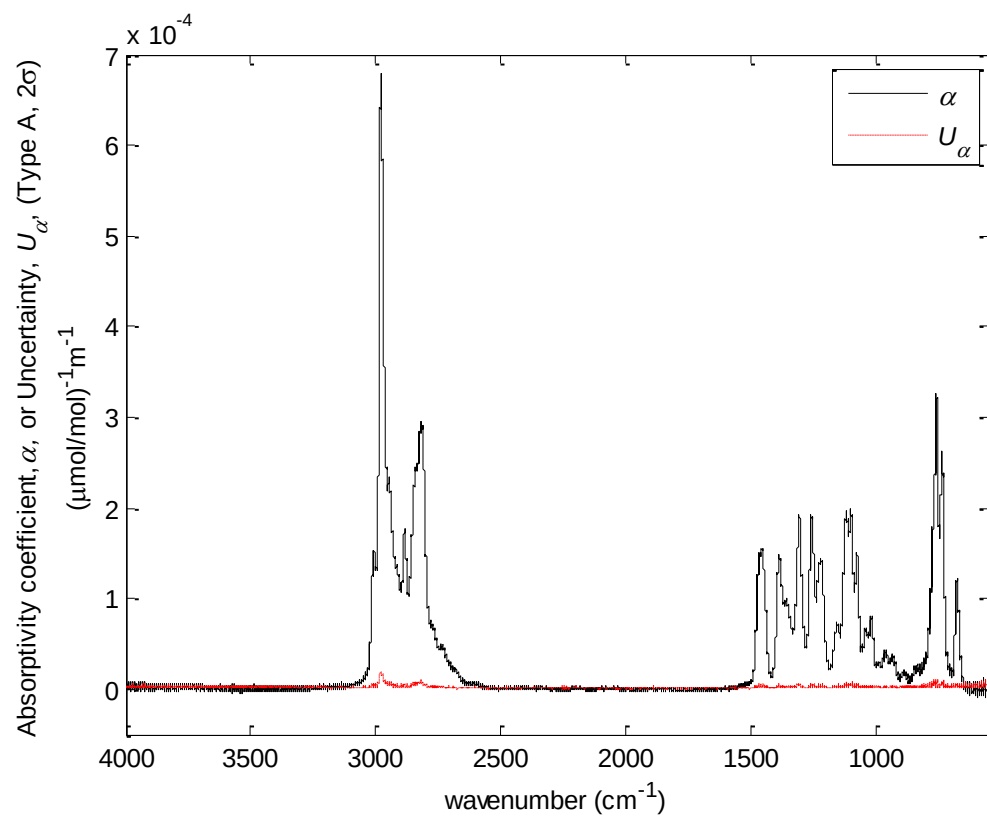


Figure 2. Plot showing (black) absorptivity coefficient and (red) statistical uncertainty (Type-A, 2σ) of HN1.

Table 4. Absorptivity Coefficient of HN1 at Selected Points

Position of Peak		Absorptivity Coefficient	
cm^{-1}	μm	$(\mu\text{mol/mol})^{-1}\text{m}^{-1}$	$(\text{mg/m}^2)^{-1}$
675.489	14.804	1.183E-04	1.680E-05
736.241	13.583	2.581E-04	3.665E-05
756.903	13.212	3.203E-04	4.547E-05
1018.517	9.818	7.749E-05	1.100E-05
1042.056	9.596	6.305E-05	8.953E-06
1076.154	9.292	1.480E-04	2.102E-05
1100.156	9.090	1.944E-04	2.761E-05
1118.554	8.940	1.946E-04	2.764E-05
1156.227	8.649	7.026E-05	9.977E-06
1221.870	8.184	1.434E-04	2.037E-05
1257.489	7.952	1.898E-04	2.695E-05
1307.481	7.648	1.905E-04	2.705E-05
1357.829	7.365	9.891E-05	1.405E-05
1388.403	7.203	1.456E-04	2.068E-05
1457.159	6.863	1.530E-04	2.172E-05
2818.975	3.547	2.932E-04	4.164E-05
2885.191	3.466	1.763E-04	2.504E-05
2979.765	3.356	6.742E-04	9.572E-05
3007.961	3.325	1.525E-04	2.165E-05

Expanded Type-A uncertainties (U_A) were generally 2 to 3% of the absorptivity coefficient, as shown in Figure 3. Figure 3a is a plot of absorptivity coefficients (abscissa) and fractional uncertainty (Type-A, $U_A, 2\sigma$) (ordinate scale). Figure 3b is a plot of the absorptivity coefficient and uncertainty and also includes a best fit of the data points obtained by least-squares approach, which is an approximation of $U_A \approx m\alpha + b$. For the fitted line in Figure 3b, the coefficients are $m = 1.91 \times 10^{-2}$ and $b = 1.40 \times 10^{-6}$ (Table 5).

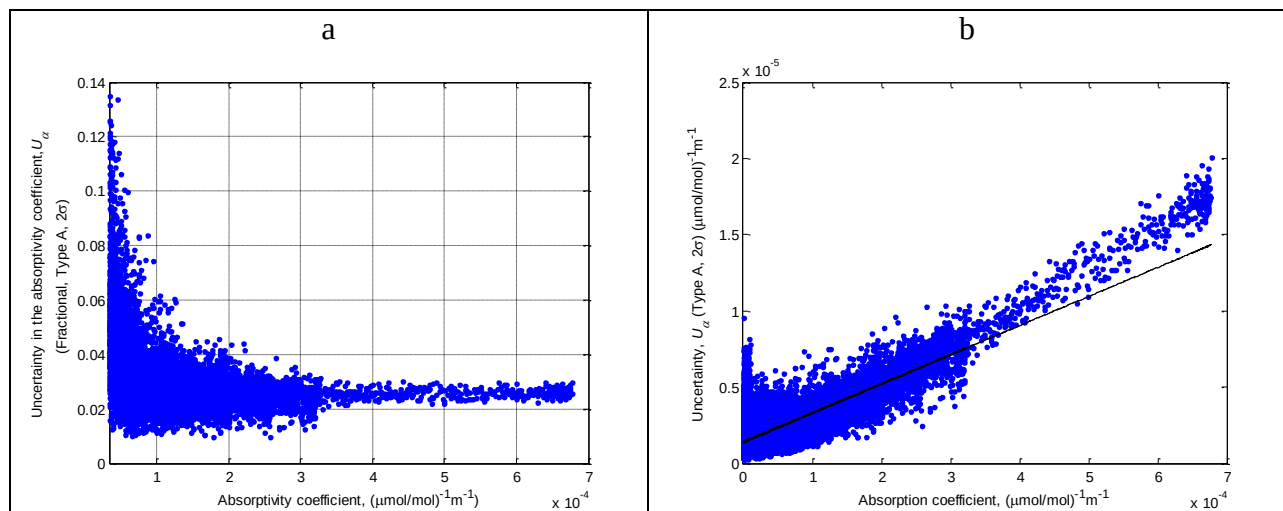


Figure 3. Statistical (Type-A) uncertainty in absorptivity coefficient spectrum of HN1. (a) Fractional uncertainty as a function of the value of α and (b) absolute uncertainty in α as a function of α . The black line represents the first-order best fit of the data points in blue, for which the coefficients are given in Table 5.

Table 5. Type-A Statistical Uncertainty for HN1 Vapor-Phase Absorptivity Coefficient

Type-A Uncertainty $2\sigma \approx ma + b$	
Slope m	Intercept b
1.91×10^{-2}	1.40×10^{-6}

Type-B estimated standard errors along with their sources, as well as the combined Type-A and B uncertainties, are provided in Table 6. The expanded combined Type-B uncertainty was computed using eq 5 (symbols defined in Table 6)

$$\Delta_B = (\Delta L^2 + \Delta T^2 + \Delta P^2 + \Delta FTIR^2 + \Delta NL^2 + \Delta MR^2 + \Delta D)^{1/2} \times 2 \quad (5)$$

Table 6. Uncertainties in Absorptivity Coefficient of HN1 from ECBC Data

Symbol	Fractional Deviation	Source
ΔL	0.005	Path length
ΔT	0.0006	Temperature of White cell
ΔP	0.002	Pressure
$\Delta FTIR$	0.0005	Drift in spectrometer
ΔNL	0.01	Nonlinearity in detector
ΔMR	0.005	Mass rate
ΔD	0.005	Dilution rate
$\Delta Purity$	0.005	Purity of feedstock
Δ_B	0.032	Combined Type-B (2σ)
Δ_A	0.021	Type-A deviation (2σ)

Notes: The Type-A uncertainty is for $\alpha = 0.000674 \text{ (}\mu\text{mol/mol)}^{-1}\text{m}^{-1}$.

For $\alpha = 0.000674 \text{ (}\mu\text{mol/mol)}^{-1}\text{m}^{-1}$, the expanded fractional uncertainty is 4.0% of the absorptivity coefficient.

The expanded Type-A uncertainty shown in Table 6 is for $\alpha = 0.0000674 \text{ (}\mu\text{mol/mol)}^{-1}\text{m}^{-1}$. As shown in Table 4, the only absorption feature with a peak maximum that strong is a C–H stretch near 2980 cm^{-1} . For values of the absorptivity coefficient less than the maximum, the fractional Type-A uncertainty is larger. For $\alpha = 0.000136 \text{ (}\mu\text{mol/mol)}^{-1}\text{m}^{-1}$, which encompasses the most intense features in the 8–12 μm region, the expanded Type-A uncertainty is 2.9% of the absorptivity coefficient.

A literature search did not identify another reference to the vapor-phase absorptivity coefficient of HN1. The complex refractive index of the compound has been measured (subject report to be published separately¹⁰) using variable-angle spectral ellipsometry. Ellipsometry was used to yield the real (n) and imaginary (k) refractive index of a compound in the condensed phase. The imaginary part of the refractive index was then computed to the linear absorptivity coefficient (K) using eq 6

$$K(\tilde{\nu}) = \frac{4\pi k(\tilde{\nu})}{\ln(10)} \quad (6)$$

The vapor-phase absorptivity coefficient (shown in Figure 2) was then transformed to a linear absorptivity coefficient. A comparison between the K -spectra of the vapor and liquid is shown in Figure 4. With the exception of the strong features between 800 and 700 cm^{-1} (very polar C–Cl stretch¹¹), the positions of the bands were similar. For C–Cl, the maximum in the vapor phase was observed near 756 cm^{-1} while for the sample in the liquid phase, the peak maximum was observed near 723 cm^{-1} . Except for the absorption band near 1450 cm^{-1} (C–H bending mode¹¹), the intensities of the bands were similar.

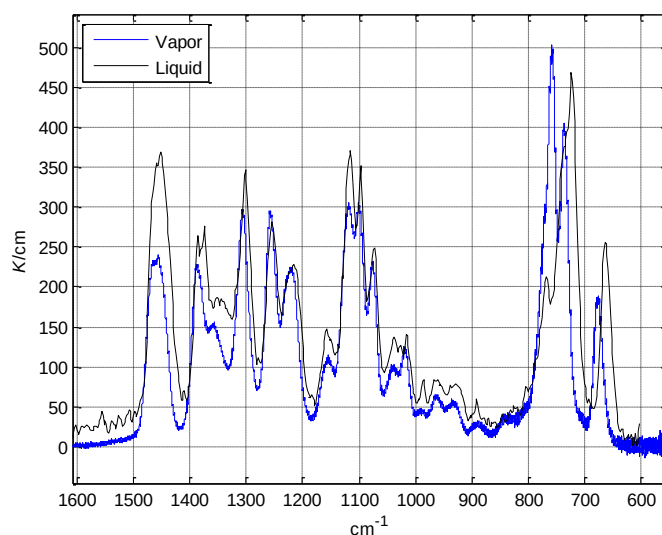


Figure 4. Linear absorptivity coefficients of HN1 showing (blue) vapor and (black) liquid.

4. CONCLUSIONS

We used a saturator cell system to acquire a series of vapor-phase IR spectra of the vesicant *bis*-(2-chloroethyl)ethylamine (HN1) in the range of 4000 to 550 cm^{-1} . The spectra were then used to compute the vapor-phase absorptivity coefficient of the compound. Expanded uncertainties in the data were Type-A at 2.1% and Type-B at 3.2%. To our knowledge, no independent measurements of the vapor-phase absorptivity coefficient of the compound were available for comparison at the time of this study. Positions and intensities of the absorption features in the vapor-phase spectrum of HN1 were similar to those in the spectrum of the liquid form, which was acquired in the ECBC laboratory using an ellipsometric technique.

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ACRONYMS AND ABBREVIATIONS

^{13}C -NMR	carbon-13 nuclear magnetic resonance (spectroscopy)
CAS RN	Chemical Abstracts Service Registry Number
CL	concentration–path length
frac	fractional statistic
ECBC	U.S. Army Edgewood Chemical Biological Center
FTIR	Fourier transform infrared spectrometer
GC	gas chromatography
HD	sulfur mustard
HeNe	helium–neon (laser)
HgCdTe	mercury–cadmium–telluride detector
HN1, HN2, HN3	nitrogen mustards
MS	mass spectrometry
TCD	thermal conductivity detection

