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VAPOR PRESSURE OF N-NITROSODIMETHYLAMINE

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Aerospace Corporation

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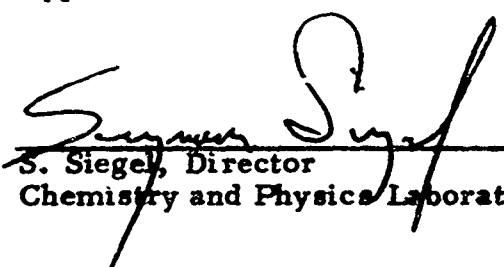
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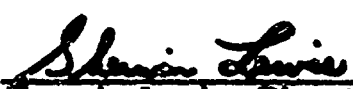
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The vapor pressure of N-nitrosodimethylamine, NDMA, from 0 to 40°C has been measured. Equations have been derived for the equilibrium vapor pressure and for the standard Gibbs energy of vaporization as functions of temperature. The pertinent thermodynamic properties ΔG° , ΔH° , and ΔS° at 298.15 K have been presented.		

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I. INTRODUCTION

N-nitrosodimethylamine, NDMA, has been reported to be carcinogenic to animals.¹⁻³ Nitrosamines are easily produced by chemical and bacterial action on secondary amines in the presence of nitrites. NDMA has been found in foods, soil, and some industrial waste solutions.⁴⁻⁶ Accidental spilling of NDMA and disposal of waste solutions containing NDMA may present serious health and environmental hazards. In order to calculate the possible level of NDMA contamination in spilling and in the disposal of waste solutions, it is necessary to know the vapor pressure of NDMA as a function of temperature. There are no reliable data on the vapor pressure of NDMA. The only value, about 5 mm at room temperature, was estimated by Bamford⁷ in 1939. The vapor pressure of NDMA was measured from 0 to 40°C in this investigation.

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II. EXPERIMENTAL PROCEDURE

The static method of vapor pressure measurement was used in this investigation. The apparatus was a conventional manometric type (Fig. 1). A sample bulb, approximately 10 cm^3 , was connected to a mercurial manometer of 8 mm o.d. and 150 mm length. A glass-coated magnetic bar was placed in the sample bulb for stirring the liquid sample. Both sides of the manometer could be evacuated either separately or simultaneously through Stopcocks A, B, and C (Fig. 1).

The general procedure for a vapor pressure determination was as follows: A 5-cm^3 sample of liquid, better than 99% pure* (Eastman Organic Distillation Products), was injected into the bulb with a syringe. The bulb and manometer assembly was attached to a vacuum line by a clamped ball and socket joint at D. In order to expel the air in the system and the dissolved gases in the liquid, the following procedure was adopted. The liquid sample in the bulb was frozen with liquid nitrogen, and the entire system was evacuated thoroughly by a vacuum pump with a liquid nitrogen trap. The sample was isolated from the rest of the system by closing Stopcock C. The sample was then melted, stirred, and evacuated for a few seconds by opening and closing Stopcock C. Stopcock C was closed, and the sample was frozen. The bulb was evacuated again. While the sample was still frozen, Stopcock C was closed and the entire bulb and manometer assembly was submerged to Stopcock A in a thermostatic bath. The other side of the manometer was evacuated continuously through Stopcocks A and B. Manometric readings were taken until equilibrium was reached, usually 10 to 15 min. The sample side was evacuated for a few seconds, and the manometric readings were taken again. The process of evacuating and reading was repeated until reproducible equilibrium readings were obtained.

* M. H. Mach, Chemistry and Physics Laboratory, The Aerospace Corporation, determined this value by means of gas chromatography mass spectrometry.

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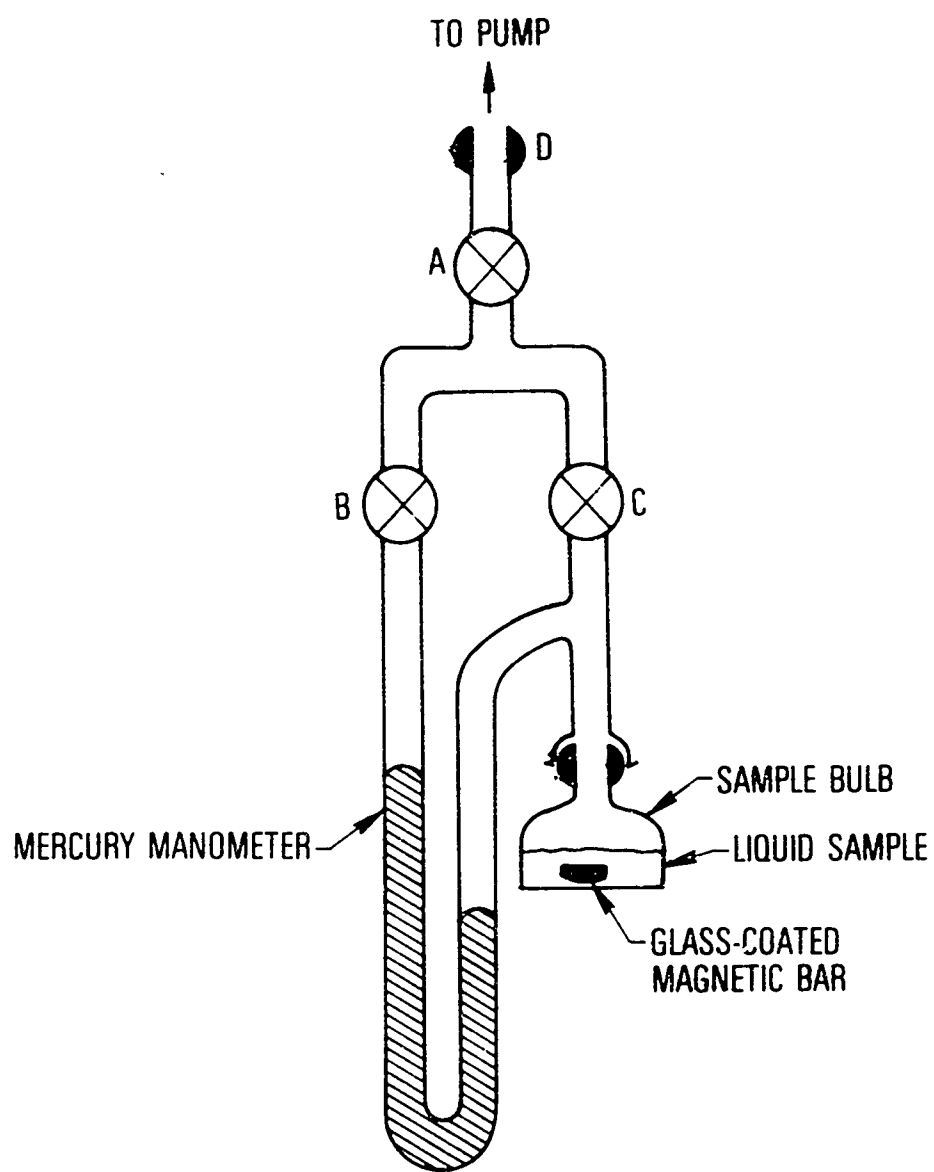


Fig. 1. Apparatus for Vapor-Pressure Measurement

The manometer was read to within ± 0.01 mm with a precision cathetometer. The thermostatic bath temperature was measured with a calibrated thermometer to $\pm 0.02^\circ\text{C}$. The accuracy of the foregoing experimental procedure was checked previously by using pure water; the vapor pressure of water was obtained within 0.3% of the published value of 23.76 Torr at 25°C .

III. RESULTS

The results for the vapor pressure measurements of NDMA from 0 to 40°C are presented in Table 1. A plot of $\log_{10} P'$ (mm Hg) versus $10^3/T$ in K^{-1} for NDMA is shown in Fig. 2. The linear equation for the vapor pressure of NDMA as a function of temperature is

$$\log_{10} P' \text{ (mm Hg)} = - \frac{2537}{T} + 9.415 \quad (1)$$

The constants in Eq. (1) are obtained by the method of least squares. The data are represented by Eq. (1) with an average deviation of $\pm 3.7\%$.

Table 1. Vapor Pressure of NDMA

t (°C)	P' (mm Hg)
0	1.28
10.1	2.96
20.0	6.21
30.0	10.90
39.5	19.54
40.0	19.50

The standard Gibbs energy of vaporization, ΔG° , is obtained by

$$\Delta G^\circ = - RT \ln P \text{ (atm)} = - 4.5756 T \log_{10} P \text{ (atm)} \quad (2)$$

substitution into Eq. (1); the result is

$$\Delta G^\circ = 11,608 - 29.90 T \quad (3)$$

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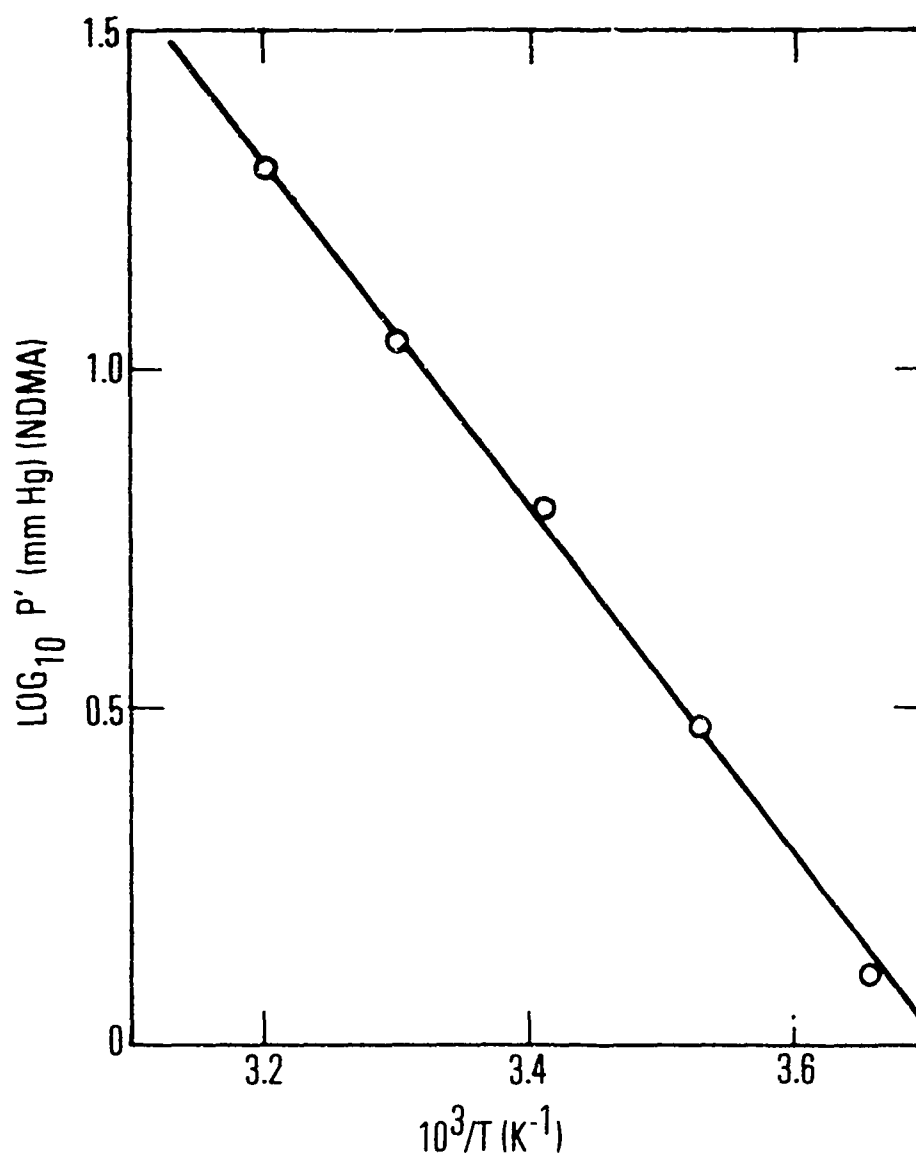


Fig. 2. Vapor Pressure of NDMA

The standard enthalpy and entropy of vaporization are obtained by the thermodynamic relation

$$\Delta G^{\circ} = \Delta H^{\circ} - T \Delta S^{\circ} \quad (4)$$

where the superscript o represents 1 atm as the standard state for each phase of the pure component. The relevant thermodynamic properties of NDMA at 25°C are as follows:

1. Standard Gibbs energy of vaporization

$$\Delta G_{298.15}^{\circ} = -2,693 \text{ cal/mol}$$

2. Enthalpy of vaporization

$$\Delta H_{298.15}^{\circ} = 11,608 \text{ cal/mol}$$

3. Entropy of vaporization

$$\Delta S_{298.15}^{\circ} = 29.90 \text{ cal/mol K}$$

It is assumed that ΔH° and ΔS° are independent of temperature over the temperature range 0 to 40°C.

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