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VAPOR PRESSURE OF  
METHYLPHOSPHONIC DICHLORIDE:  
A COMPENDIUM

by Ann Brozena  
Donald Fielder  
RESEARCH DIRECTORATE

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PREFACE

The work described in this report was authorized under Project 1L162706A553, Deterrent Systems. This work was started in May 1984 and completed August 1984. The experimental data are recorded in laboratory notebook 83-0149.

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VAPOR PRESSURE OF METHYLPHOSPHONIC DICHLORIDE:  
A COMPENDIUM

1. INTRODUCTION

Vapor pressure data for the compound methylphosphonic dichloride (hereafter called dichlor) can be found in many sources, both open literature and unpublished reports. This report attempts to consolidate all available data, evaluate it, and develop a best-fit predictive Antoine equation for the combined data.

2. DATA SOURCE

<sup>cont'd</sup> Zeffert published an Antoine equation for dichlor in 1960. However, no experimental data were given in the report. Several British technical reports contained some experimental vapor-pressure data for dichlor, and several Edgewood Arsenal contractor reports also contained vapor-pressure data for the compound. The data from these various sources were combined into a set and evaluated, using Penski and Latour's method of computation. Zeffert's equation was used to calculate values for his experimental data and these values were used when all data were combined into a set.

3. EVALUATION OF DATA

When the combined data were evaluated by Penski and Latour's method, an arbitrary limit of 10-percent difference between the experimental and the calculated value was chosen as the criteria for excluding a member from the set. Using this criteria, 10 members of the set were deleted as being out of range. The final set contained 57 members of which 14 were calculated from Zeffert's equation. This set of values was then used to calculate the Antoine vapor-pressure equation of the form.

$$\log_{10}P = A - \frac{B}{(C+t)} \quad (1)$$

where

P = vapor pressure in torr  
t = temperature in degrees centigrade  
A, B, C = constants

The standard deviation, SD, was calculated for the Antoine equation using the following equation:

$$S.D. = \left( \frac{s}{n-1} \right)^{1/2} \quad (2)$$

where

$$s = \sum \left( \log_{10} P_{\text{calc}} - \log_{10} P_{\text{exp}} \right)^2$$

The logarithmic values were used since it has been reported<sup>12</sup> that this procedure prevents excess weighting of the higher vapor-pressure data.

The constants derived for the Antoine equation were used to calculate the heat of vaporization in kcal/mole and the volatility in g/m<sup>3</sup> at various temperatures from the following respective equations:

$$\Delta H_{\text{vap}} = 2.303 RB \left( \frac{T}{C+t} \right)^2 \quad (3)$$

$$\text{Volatility} = \frac{PM}{760R^1T} \quad (4)$$

where

- B & C = Antoine equation constants
- t = temperature in degrees centigrade
- T = temperature in degrees Kelvin
- P = vapor pressure in torr
- M = molecular weight in g/mole
- R = gas constant
- =  $1.987 \times 10^{-3}$  kcal/g-mole<sup>o</sup>K
- R<sup>1</sup> = gas constant
- =  $82.05 \times 10^{-6}$  atm-m<sup>3</sup>/g-mole<sup>o</sup>K

#### 4. DISCUSSION

At the top of table 1 are shown the A, B, and C Antoine constants, the standard deviation of the equation, and the calculated boiling point. This table lists the experimental and calculated vapor pressures and the percent difference between the two for dichlor at various temperatures. Table 2 contains the calculated volatility and heat of vaporization as a function of temperature. The figure shows a plot of the vapor pressure (torr) versus 1/T K; the line is calculated and the points are experimental. The data are in good agreement considering that they are from many sources. Additionally, the boiling point calculated from this data compilation closely agrees with that obtained by Hofmann<sup>13</sup> in 1873 (165<sup>o</sup> versus 163<sup>o</sup>C).

## 5. CONCLUSION

Vapor-pressure data for dichlor from many sources has been reviewed and analyzed to obtain a best-fit predictive Antoine equation. The data shows internal consistency and no large deviations.

Table 1. Experimental and Calculated Vapor Pressures for Dichlor

Antoine Constants			
A = 7.51821			
B = 1831.49			
C = 229.687			
Standard Deviation 0.0103			
Calculated Boiling Point 165.3°C			
Temperature (°C)	Vapor Pressure (torr)		Percent Difference
	Experimental	Calculated	
39	5.0	5.03	0.65
47	8	7.92	-0.97
50	9.3	9.33	0.32
50	10.1	9.33	-7.63
60	15.7	15.70	0.00
60	15.5	15.70	1.29
60.5	15	16.10	7.33
62	18	17.35	-3.62
64.5	18.5	19.62	6.03
65	20	20.10	0.50
70	25	25.52	2.08
70	25.6	25.52	-0.32
70	26.7	25.52	-4.42
74	30	30.72	2.38
80	40	40.20	0.50
80	40.3	40.20	-0.25
84.0	47.0	47.82	1.75
85.5	50	50.98	1.96
90	61.6	61.55	-0.09
90	63.1	61.55	-2.46
92.0	67.0	66.81	-0.29
95	75	75.41	0.55
99.0	88.0	88.32	0.37
100	91	91.83	0.91
100	91.6	91.83	0.25
100	92	91.83	-0.19
102.5	100	101.11	1.11
105.5	113.0	113.27	0.24
108	125	124.33	-0.54



Table 1. (Continued)

Temperature (°C)	Vapor Pressure (torr)		Percent Difference
	Experimental	Calculated	
110	133.0	133.82	0.61
110	137.4	133.82	-2.61
111.5	144.0	141.32	-1.86
112.5	150	146.52	-2.32
117.5	175	174.98	-0.01
118.0	179.0	178.06	-0.52
120	188.9	190.85	1.03
120	192	190.85	-0.60
121.5	200	200.94	0.47
122	210.6	204.40	-2.94
124.0	218.0	218.74	0.34
128	250	249.94	-0.02
130	262.9	266.88	1.51
130	265	266.88	0.71
132.0	282.0	284.75	0.98
133	300	294.06	-1.98
140	359.2	366.48	2.03
142	400	389.68	-2.58
150	500	494.91	-1.02
150	482.4	494.91	2.59
150	519.3	494.91	-4.70
156	600	588.26	-1.96
160	637.8	658.13	3.19
162	700	695.52	-0.64
165	750.5	754.83	0.58
165	758	754.83	-0.42
165.5	760	765.10	0.67
167	768.8	796.61	3.62

Table 2. Calculated Volatility and Heat of Vaporization  
at Selected Temperatures

Temperature (°C)	Volatility (g/m <sup>3</sup> )	Heat of Vaporization (kcal/mole)
35.0	27.46	11.36
40.0	36.30	11.30
45.0	47.50	11.24
50.0	61.53	11.19
55.0	78.97	11.14
60.0	100.44	11.08
65.0	126.68	11.04
70.0	158.50	10.99
75.0	196.81	10.94
80.0	242.60	10.90
85.0	297.00	10.86
90.0	361.21	10.81
95.0	436.57	10.77
100.0	524.49	10.74
105.0	626.54	10.70
110.0	744.38	10.66
115.0	879.78	10.63
120.0	1034.64	10.59
125.0	1210.97	10.56
130.0	1410.89	10.53
135.0	1636.64	10.50
140.0	1890.55	10.47
145.0	2175.08	10.44
150.0	2492.77	10.41
155.0	2846.27	10.38
160.0	3238.33	10.35
165.0	3671.78	10.33

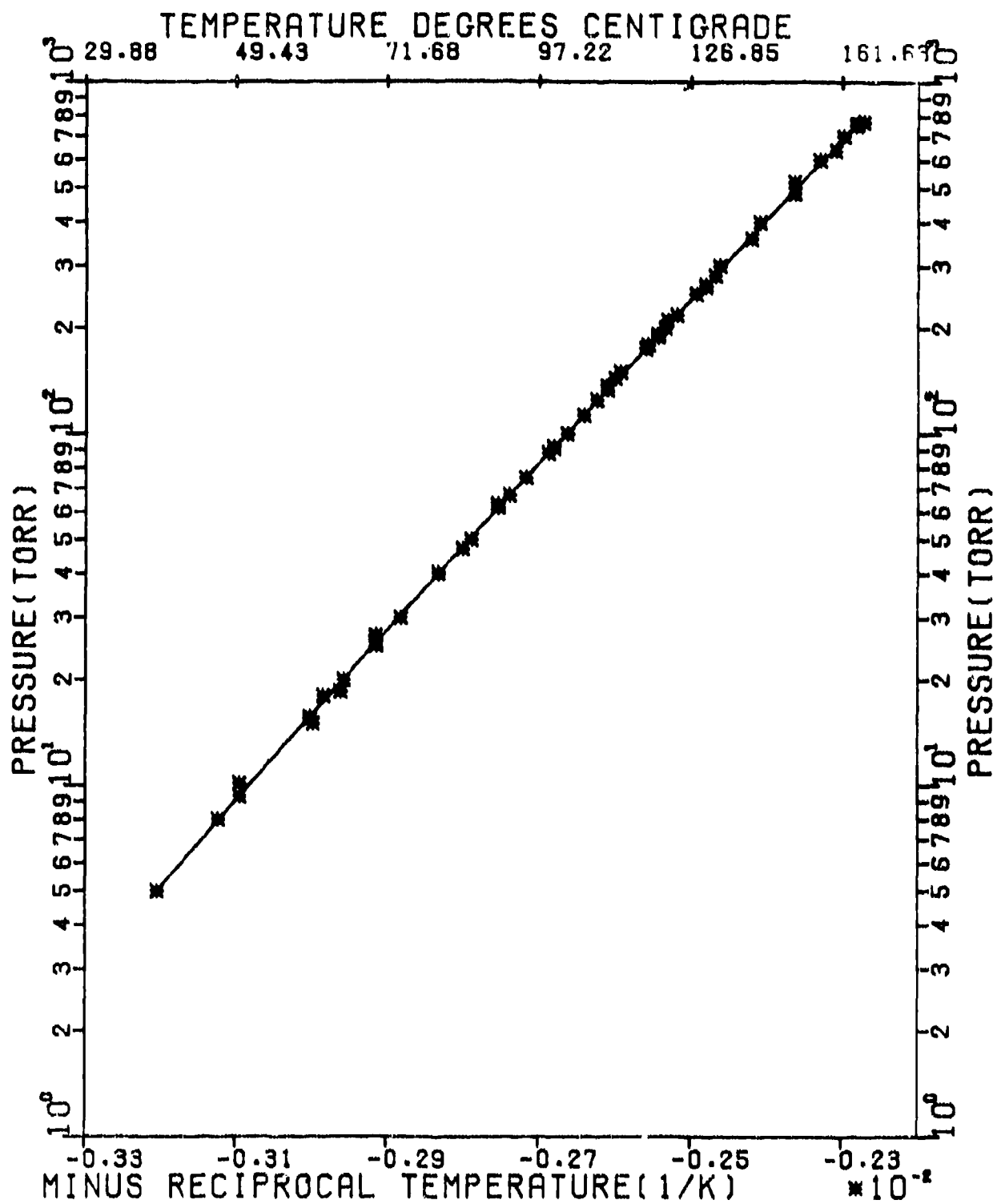


Figure. Plot of Vapor Pressure of Methylphosphonic Dichloride

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