REPORT NO. DOT/MTB/OHMO-75/4

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TOXIC POINT DETERMINATION OF SELECTED HAZARDOUS MATERIALS

LEVEL II

RICHARD A. DAVIS
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DECEMBER 1975

FINAL REPORT

PREPARED FOR
DEPARTMENT OF TRANSPORTATION
MATERIALS TRANSPORTATION BUREAU
Office of Hazardous Materials Operations
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16. Abstract

"Toxic Point" is a term under consideration by the United Nations of Rapporteurs on the Packaging of Dangerous Goods. It is defined the temperature at which the equilibrium concentration of vapor of substance measured at 760 millimeters is equal to the LC50 of the substance. This is also referred to as the "Temperature Threshold Toxicity"

This report contains the "Toxic Points" calculated for 57 substanc The calculations are shown together with the toxicity and vapor pressure data used therein.

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INTRODUCTION

This report contains the toxic points for 57 of the 85 compounds requested by the Department of Transportation, Materials Transportation Bureau. An extensive search was conducted to obtain vapor pressure and one-hour rat LC_{50} data. There were many compounds for which no usable rat inhalation toxicity data (LC_{50}'s) could be found. Consequently, other available rat LD_{50} data were used to estimate an LC_{50} figure while taking into account the route of administration. When such information was not available for the rat, LC_{50} or LD_{50} values from other species were used. The toxic points computed from rat data are listed in Table I. The toxic points computed for other species are listed in Table II.

A toxic point determination was not possible for the following compounds due to unavailable vapor pressure or toxicity information.

No Vapor Pressure Data	No Toxicity Data
Allylamine	Allyl Ethyl Ether
Chloroacetaldehyde	Antimony Pentafluoride
4-chloro-o-toluidine Hydrochloride	Arsenic Trichloride
Diallyl Ether	Benzotrichloride
Diethylenetriamine	Bromoacetone
Ethylchloroformate	Chloroacetone
Ethyleneimine	Chloroprene
Hexaethyltetraphosphate	Cyanogen Bromide
Methacrylaldehyde	Diphenylchloroarsine
Methylchloroformate	Ethyldichloroarsine
Methyl Chloromethyl Ether or Chloromethyl Methyl Ether	Methyl Bromide
Perchloromethylmercaptan	Nitroanisole
	Nitrobenzotrifluoride
	Nitrobromobenzene
	Nitroxylene
	Pentachloroethane
	Phenetidine
	1,1,2,2-Tetrachloroethane
	Xylyl Bromide

METHODS

Estimation of The One-Hour LC_{50}

The one-hour rat LC_{50} was estimated from a rat LC_{50} of different duration by multiplying the different duration LC_{50} by the factor $\frac{\text{duration (hours)}}{\text{1 hour}}$. If no rat LC_{50} could be found, a rat LD_{50} was used to calculate an estimated one hour LC_{50} using the equation shown below:

$$\text{Estimated } LC_{50} = \frac{LD_{50}\ (\text{mg/Kg}) \times \text{Average Rat Body Weight (0.2 Kg)}}{\text{Avg Rat Min Vol } (10^{-4}\text{m}^3/\text{min}) \times 60 \text{ Min} \times \text{Absorption Factor (0}$$

The units of the estimated LC_{50} are mg/m^3 which are converted to parts per million (ppm) using the formula:

$$\text{ppm (by volume)} = \frac{24.45 \times mg/m^3}{\text{Molecular Weight}}$$

The vapor pressure equations described below require that the LC_{50} be expressed as a vapor pressure in millimeters mercury (mm Hg). This was done using the following equation:

$$\text{mm Hg} = \frac{\text{ppm}}{10^6} \times 760$$

Calculation of Toxic Points

Toxic points were calculated by substituting the vapor pressure in mm Hg which corresponded to the one-hour rat LC_{50} into one of the following equations:

1. $\text{Log}_{10}P = -\frac{0.2185\ A}{T} + B$

   where P is the vapor pressure in mm Hg
   T is the temperature in degress Kelvin
   A is the molar heat of vaporization in calories per gram mole
   B is a constant

2. $\text{Log}_{10}P = A - \frac{B}{t + c}$

   where P is the vapor pressure in mm Hg
   t is the temperature in degrees centrigrade
   A, B and C are constants

If the values for A, B and C could not be found for one of these equations, then the constants for equation 2 were calculated. The preferred method of calculating A, B and C was described by Thomson (Chemical Reviews 38:1-39, 1946) and requires the temperature and pressure of three widely separated boiling points. The equations used are as follows:

$$\frac{y_3 - y_2}{y_2 - y_1} \times \frac{t_2 - t_1}{t_3 - t_2} = 1 - \frac{t_3 - t_1}{t_3 + C}$$

$$B = (t_1 + C)\ (t_3 + C) \times \frac{y_3 - y_1}{t_3 - t_1}$$

$$A = y_1 + \frac{B}{t_1 + C}$$

where: y_1, y_2 and y_3 equal Log P_1, Log P_2 and Log P_3, respectively; P representing the pressures (mm Hg) at which the different boiling points occur. t_1, t_2 and t_3 are the temperatures in degrees centigrade of the different boiling points.

If the boiling points are inaccurate or not widely separated, the calculated value of C can be in considerable error and not usable. In this case C was calculated from the equation

$$C = 239 - 0.19t_{760}$$

where t_{760} is the boiling point at 760 mm Hg pressure in degrees centigrade. If only two boiling points could be found for a compound, the value of C was set at 230.

Whenever the values for A, B and C had to be calculated, the values were checked by showing that equation 2 produced the same temperatures and pressures of the boiling points used to calculate A, B and C.

TABLE I
TOXIC POINTS DERIVED FROM RAT DATA

COMPOUND	TP	LC_{50}		BP		VAPOR PRESSURE CONSTANTS			
	°C	PPM	REF.	°C	REF.	A	B	C	REF.
Cyanogen Chloride	-144.8	59	4a	12.7	12	5243.4	7.541733		12
Nickel Carbonyl	-115.5	17	1a	43.0	11	7021.2	7.738785		12
Chlorine Trifluoride	-110.4	380	1	11.8	11	5932.4	7.436405		12
Acrolein	-97.2	32	1a	52.5	11	7.00995	1175.6	232.2	9*
Ammonia (Anhydrous)	-96.8	7338	1	-33.4	11	7459.6	9.997400		12
Hydrogen Fluoride	-94.9	1276	4	19.7	11	6018.2	7.370000		12
Boron Trichloride	-83.8	3480	13	12.5	11	6165.6	7.543306		12
Nitrogen Tetroxide	-72.6	115	1	8.1	10	†			10
Iron Pentacarbonyl	-65.6	56	1a	103.0	11	8985.8	8.067387		12
Bromochloromethane	-61.4	465	2	68.1	6	6.86624	1132.3	216	6
Methylhydrazine	-48.1	296	4a	87.5	7	7.39188	1403.1	222.4	7*
Acrylonitrile	-44.2	2434	4c	78.5	8	7941.4	7.851016		12
Propionitrile	-40.0	947	4f	97.1	8	8769.0	8.079473		12
Ethyl Bromide	-36.5	26980	1	38.4	8	6843.1	7.635277		12
Chloroform	-35.4	9026	4f	61.3	8	7500.5	7.735083		12
Methylene Chloride	-28.7	33868	4f	40.7	8	7572.3	8.183300		12
Chloropicrin	-20.4	2053	4f	112.0	11	9109.7	8.072388		12
Ethylene Dibromide	-19.9	689	3	131.4	6	7.06245	1469.7	220	6
1,1,2,2-Tetrachloroethylene	-18.6	1624	2f	120.8	8	9240.5	8.026207		12
Allyl Alcohol	-17.7	1620	1	96.9	8	10577.7	9.143231		12
Epichlorohydrin	-17.3	1316	4f	117.9	8	9815.4	8.388568		12
1,1,1,2-Tetrachloroethane	-14.3	1605	4f	130.5	8	9296.5	7.938042		12
Carbon Tetrachloride	-13.6	19056	1	76.6	8	7628.8	7.586045		12
Hydrazine	-5.3	2280	4a	113.5	7	7.55350	1551.4	217.4	7*
Ethylenechlorohydrin	-3.3	1408	4c	128.8	8	10740.6	8.730379		12
Isothio-Cyanic Acid Allyl Ester	5.4	2013	4f	150.7	8	9967.8	8.007150		12

TABLE I (Continued)
TOXIC POINTS DERIVED FROM RAT DATA

COMPOUND	TP	LC_{50}		BP		VAPOR PRESSURE CONSTANTS			
	°C	PPM	REF.	°C	REF.	A	B	C	RE
Trichloroethylene	12.1	50434	4f	87.2	8	8314.7	7.956342		1
Dichloroethyl Ether	13.6	710	4f	178.0	11	11376.8	8.405945		1
Pyridine	17.3	16000	4a	115.2	8	9649.4	8.347670		1
Aniline	23.2	1000	1a	184.4	8	11307.6	8.221995		1
Dimethyl Sulfate	25.8	1066	4b	188	11	7.629081	1974.6	230	1
Acetonitrile	26.5	124724	4f	81.6	11	8173.2	7.938662		1
Mesityl Oxide	28.9	15382	4f	129.8	8	10109.4	8.383703		1
Toluene Diisocyanate (TDI)	34.8	56	4a	251.0	11	8.11948	2519.8	230	1
Ethylenediamine	36.4	32000	4a	116.5	11	7.91721	1777.8	235.8	
1,2-Dichlorobenzene	39.8	4579	3f	179.0	8	10943.0	8.185275		1
Ester Isocyanophenyl ...	45.1	10632	4f	165.6	8	10556.7	8.159059		1
2-Chlorophenol	46.4	9960	4c	174.5	8	10341.1	7.952334		
Ethyl Sulfate (Diethyl)	59.7	2974	4b	208.0	12	12518.2	8.574200		
1,2,4-Trichlorobenzene	64.3	5605	4f	213.0	8	11425.1	8.030523		
1,4-Dichlorobenzene	66.3	22908	4e	173.9	6	10611.0	8.073632		
Acetocyanohydrin	66.8	248	1a	95.0	11	39.6536	11620.2	221	
Benzonitrile	72.9	15671	4d	191.3	8	11341.0	8.239760		
Chloronitrobenzene (Ortho)	75.2	2461	4f	245.5	11	7.55514	2222.6	230	
o-Toluidine	79.4	11316	4f	199.8	8	12663.4	8.785945		
m-Toluidine	81.0	12237	4f	202.9	8	12104.1	8.440371		
Nitrotoluene (Ortho)	85.3	8750	4f	220.4	8	12239.1	8.286642		
p-Toluidine	86.2	16145	3f	200.4	8	12428.6	8.648585		
Benzylidene Chloride	96.1	27184	4f	214.0	8	11075.9	7.871695		
Diethylaniline	105.7	24263	4f	216.3	8	12539.2	8.501130		

TABLE I (Continued)
TOXIC POINTS DERIVED FROM RAT DATA

1. * - Vapor pressure constants mathematically derived from boiling points.

2. The following letters indicate an estimated one-hour LC_{50} and the type of data on which it is based. Numbers indicate the reference source.

   a = inhalation duration other than one hour
   b = intravenous LD_{50}
   c = subcutaneous LD_{50}
   d = skin LD_{50}
   e = intraperitoneal LD_{50}
   f = oral LD_{50}

3. † - The equation used to calculate the TP of nitrogen tetroxide was

$$\ln P = 32.1662156 - \frac{7788.62341}{T} + \frac{172043.271}{T^2}$$

TABLE II

TOXIC POINTS DERIVED FROM OTHER THAN THE RAT DATA

COMPOUND		TP	LC_{50}		BP		VAPOR PRESSURE CONS		
		°C	PPM	REF.	°C	REF.	A	B	
Allylchloride	(M)	-62.7	2734	4e	44.6	8	7386.8	7.991952	
Carbon Disulfide	(R)	-58.0	5303	2c	46.5	11	6786.8	7.502434	
Butyronitrite	(R)	8.7	9737	4d	117.5	8	9462.9	8.207895	
Methylchloroform	(GP)	14.3	95618	4f	74.1	8	8012.7	7.955902	
Carbon Tetrabromide	(M)	20.5	1211	4c	[illegible].5	8	10771.4	7.983739	
Bromoform	(M)	28.8	9697	4c	150.5	8	7.30383	1720.6	2
Acetylene Tetrabromide	(GP)	67.5	1553	4f	240.5	12	12911.5	8.357191	

1. * - Vapor pressure constants mathematically derived from boiling points.

2. The following letters indicate an estimated one-hour LC_{50} and the type of data on which it is based. Numbers indicate the reference source.

   a = inhalation duration other than one hour
   b = intravenous LD_{50}
   c = subcutaneous LD_{50}
   d = skin LD_{50}
   e = intraperitoneal LD_{50}
   f = oral LD_{50}

3. (M) = Mouse
   (R) = Rabbit
   (GP) = Guinea Pig

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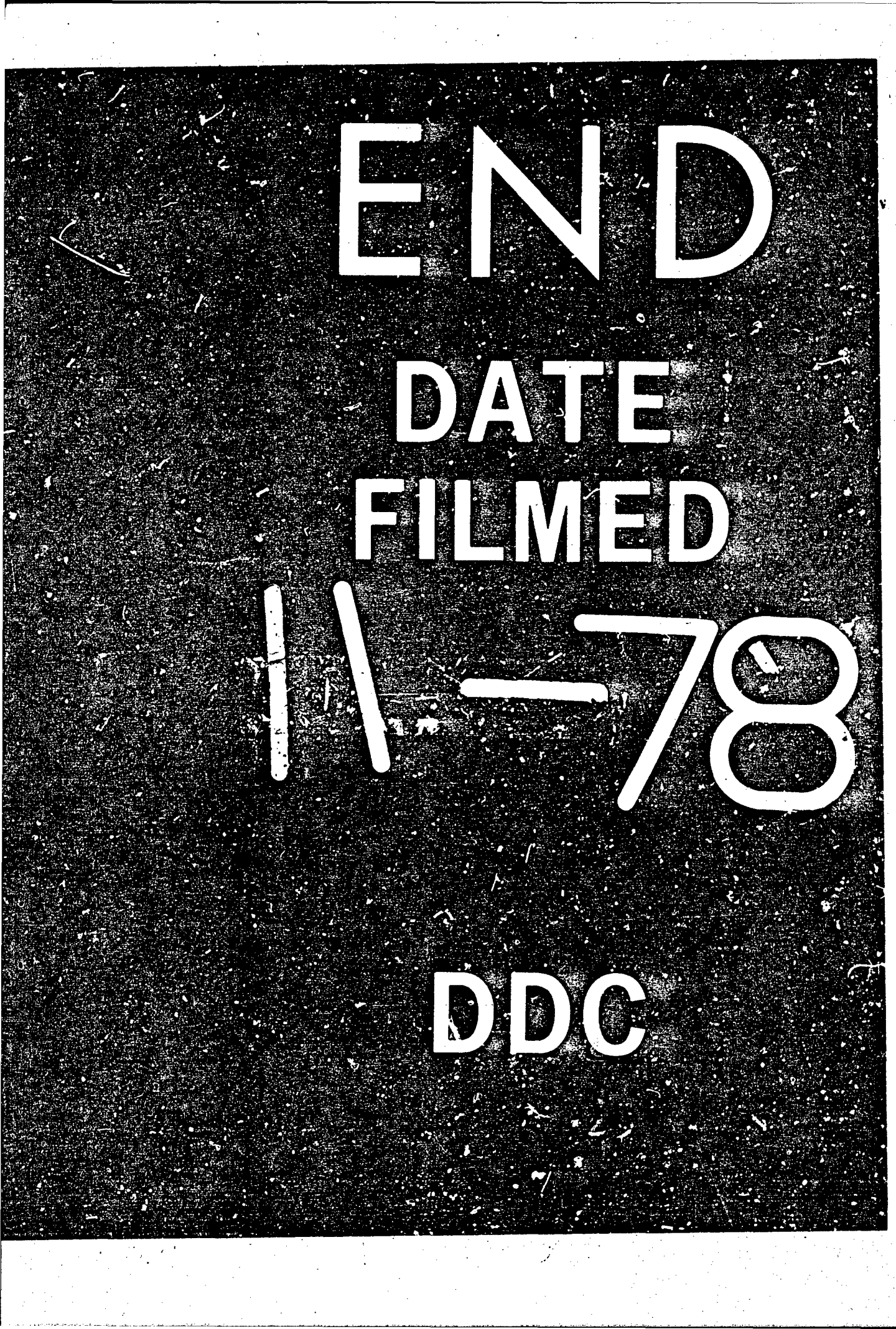
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