3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of Stoddard solvent is located in Table 3- 1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of Stoddard solvent is located in Table 3-2.

Stoddard solvent is a petroleum distillate mixture of C_7-C_{12} hydrocarbons. The mixture consists of three major groups of components: linear and branched alkanes, also known as paraffins (30-50% of the total mixture); cycloalkanes, also called cycloparaffins or naphthenes (not to be confused with naphthalenes which are bicyclic aromatics) (30-40%), and aromatic hydrocarbons (l0-20%) (Air Force 1989b; McDermott 1975). Stoddard solvent is a refinery blend of differently treated oil fractions. Its composition varies somewhat, depending on the refinery and the time of production. Table 3-3 lists some of the major components of several Stoddard solvent formulations. Petroleum distillates are often distinguished by boiling or distilling temperatures. Stoddard solvent has a boiling range of 150-200°C (Scott et al. 1959). The 140 flash Stoddard solvent is composed of C_5-C_{12} hydrocarbons and has a boiling range of 185-207°C (Air Force 1989b). White spirits is a term somewhat synonymous with Stoddard solvent since it has a hydrocarbon range between C_7 and C_{11}. Six types of white spirits have been identified based on origin. Each type consists of the same components, but the percentages vary (Scheffers et al. 1985). Possible contaminants of Stoddard solvent include lead (<1 ppm) and sulfur (3.5 ppm) (Suntech 1978).

There are a number of related chemical mixtures with components that are different from those of Stoddard solvent. For instance, high-flash aromatic naphtha is a generic term for petroleum distillates primarily consisting of C_9 aromatics (70-80%) with C_8 or C_{10} aromatics comprising the rest. Stoddard solvent, in contrast, is only l0-20% aromatic (Clark et al. 1989b; Schreiner et al. 1989). Naphtha is also a general term for petroleum distillates containing predominantly C_5-C_{13} aliphatic hydrocarbons and distilling at 30-238°C (Tenenbein et al. 1984).

TABLE 3-1. Chemical Identity of Stoddard Solvent

Characteristic	Information	Reference
Chemical name	Stoddard solvent	Sax and Lewis 1989
Synonym(s)	Dry cleaning safety solvent, naphtha safety solvent, PD-680, petroleum solvent, spotting naphtha, varnoline, white spirits	Air Force 1989b; NIOSH 1989; Sax and Lewis 1989
Registered trade name(s)	Texsolve S, Varsol 1	Budavari et al. 1989; Hunter et al. 1992
Chemical formula	Not applicable[a]	
Chemical structure	Not applicable[a]	
Identification numbers:		
CAS registry	8052-41-3	Sax and Lewis 1989
NIOSH RTECS	WJ8925000	NIOSH 1990
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	1268 27	NIOSH 1990
HSDB	No data	
NCI	No data	

[a]Stoddard solvent is a mixture of C_7–C_{12} hydrocarbons primarily containing straight and branched chain alkanes (30–50%), cycloalkanes (30–40%), and alkyl aromatic hydrocarbons (10–20%) (Air Force 1989b; McDermott 1975). See also Table 3-3.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Stoddard Solvent

Property	Information	Reference
Molecular weight	144 (mean); 135–145 (range)	Air Force 1989b; Carpenter et al. 1975b
Color	Clear, colorless	Sax and Lewis 1989
Physical state	Liquid	Sax and Lewis 1989
Melting point	No data	
Boiling point	154–202°C	Air Force 1989b
	160–199°C	Coast Guard 1985
Density:		
at 20°C	0.78 g/mL	NIOSH 1990
Odor	Similar to kerosene	NIOSH 1990
Odor threshold	0.9 ppm (5.1 mg/m^3)	Carpenter et al. 1975b
	2 mg/m^3	Hastings et al. 1984
Solubility:		
Water	Insoluble	McDermott 1975
Organic solvent(s)	Absolute alcohol, benzene, ether, chloroform, carbon tetrachloride, carbon disulfide	Sax and Lewis 1989
Partition coefficients:		
Log K_{ow}	3.16–7.06	Air Force 1989b
Log K_{oc}	2.85–6.74	Air Force 1989b
Vapor pressure at 25°C	4–4.5 mmHg	McDermott 1975
Henry's law constant:		
at 20°C	4.4×10^{-4}–7.4×10^{0} atm·m^3/mol	Air Force 1989b
Autoignition temperature	232°C	Sax and Lewis 1989
Flashpoint	37.8–60.0°C	Air Force 1989b
	38–43°C	Sax and Lewis 1989
Flammability limits:		
% volume in air at 25°C	0.9–6.0	Carpenter et al. 1975b
Conversion factors:		
at 25°C and 760 mm	1 mg/L = 174.6 ppm; 1 ppm = 5.73 mg/m^3	Carpenter et al. 1975b
at 25°C	1 ppm = 5.77 mg/m^3	Air Force 1989b
Explosive limits		McDermott 1975
Lower limit	0.9%	
Upper limit	6%	

TABLE 3-3. Possible Formulations of Stoddard Solvent (Percent)

Hydrocarbons	White Spirits 1[a]	White Spirits 2[a]	White Spirits 3[a]	Stoddard solvent[b] (regular)	Stoddard solvent[b] (140 flash)	Stoddard solvent[c]	Stoddard solvent[d]	Stoddard solvent[e]
Alkanes (paraffins)	**60.0**	**61.0**	**62.8**	**30–50 (48 average)**	**60.8**	**34.9**	**41.6**	**47.7**
n-nonane	11.3	13.3	1.9					
n-decane	7.6	10.0	9.1					
methylnonanes	4.9	7.9						
2,6-dimethyloctane	2.7	4.1						
n-undecane	2.7	2.4	17.5					
dodecanes			11.6					
terdecanes			2.7					
others	30.8	23.3						
Cycloalkanes (cycloparaffins)	**39.7**	**27.3**		**30–40 (38 average)**	**35.7**		**39.5**	**37.6**
monocycloparaffins	16.3	13.7			24.5	34.9	27.9	26.0
trimethylcyclohexane	4.7	7.2						
tert-butylcyclohexane	4.5	4.0						
n-butylcyclopentane	5.0	1.3						
n-butylcyclohexane	2.1	1.2						
other cycloparaffins	23.4	13.1						
dicycloparaffins					11.2	5.0	11.6	11.6
tricycloparaffins						0.4	0.0	
acenaphthenes						0.4		
Aromatics	**0.3**	**11.7**	**17.0**	**10–20 (14.1 average)**	**3.40**		**18.9**	
alkylbenzenes				14.0	3.03	22.0	17.6	14.1
dimethylethylbenzenes	0	3.0						
n-propylbenzene	0	2.0						
ethyltoluenes	0	1.2						
1,2,4-trimethylbenzene	0	0.9						
other aromatics	0.3	4.6				1.1		
other benzenes				0.1	0.07			0.1
indans/tetralins				<1	0.3	1.8	1.3	0.5
indenes						0.1		
naphthalenes						0.2		
acenaphthalenes						0.3		
tricyclicaromatics						0.1		

[a]Adapted from Verkkala et al. (1984)
[b]Adapted from Air Force (1989b)
[c]Adapted from American Petroleum Institute (1976)
[d]Adapted from Suntech Group (1978); API 1978a
[e]Adapted from Carpenter et al. (1975b); this paper also includes a mass spectral analysis of components by carbon number within a hydrocarbon class, e.g., C_8 alkanes.

3. CHEMICAL AND PHYSICAL INFORMATION

Benzine and mineral spirits (other associated mixtures) are similar to but not exactly the same as Stoddard solvent. Benzine consists of C_5-C_9 hydrocarbons (Takeuchi et al. 1975) and boils, on average, at between 154°C and 204°C (Navarte et al. 1989). Benzine and Stoddard solvent distill at about the same temperature range, but their hydrocarbon compositions differ. Mineral spirits have a distillation range of 136-277°C. The distillation range of Stoddard solvent falls within that of mineral spirits (Mehlman and Smart 1982). Therefore, Stoddard solvent may be considered a subset of mineral spirits, but mineral spirits as a whole are not described in this profile.