

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

The chemical synonyms and identification numbers for wood creosote, coal tar creosote, and coal tar are listed in Tables 4-1 through 4-3. Coal tar pitch is similar in composition to coal tar creosote and is not presented separately. Coal tar pitch volatiles are compounds given off from coal tar pitch when it is heated. The volatile component is not shown separately because it varies with the composition of the pitch. Creosotes and coal tars are complex mixtures of variable composition containing primarily condensed aromatic ring compounds (coal-derived substances) or phenols (wood creosote). Therefore, it is not possible to represent these materials with a single chemical formula and structure. The sources, chemical properties, and composition of coal tar creosote, coal tar pitch, and coal tar justify treating these materials as a whole. Wood creosote is discussed separately because it is different in nature, use, and risk.

Information regarding the chemical identity of wood creosote, coal tar creosote, and coal tar is located in Tables 4-1 through 4-3.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Wood creosote, coal tar creosote, coal tar, and coal tar pitch differ from each other with respect to their composition. Descriptions of each mixture are presented below.

4.2.1 Wood Creosote

Wood creosotes are derived from beechwood (referred to herein as beechwood creosote) and the resin from leaves of the creosote bush (*Larrea*, referred to herein as creosote bush resin). Beechwood creosote consists mainly of phenol, cresols, guaiacols, and xylenols. It is a colorless or pale yellowish liquid, and it has a characteristic smoky odor and burnt taste (Miyazato et al. 1981). It had therapeutic applications in the past as a disinfectant, laxative, and a stimulating expectorant, but it is not a major pharmaceutical ingredient today in the United States. Beechwood creosote is obtained from fractional distillation (200–220 EC at atmospheric pressure) of beechwood or related plants. The mixture has only recently been characterized to any significant extent (Ogata and Baba 1989). Phenol, *p*-cresol, and guaiacols

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Wood Creosote

Characteristic	Information	Reference
Chemical name	Wood creosote	Merck 1989
Synonym(s)	Beechwood creosote, creosote, creasote	Merck 1989
Registered trade name(s)	Not applicable	
Chemical formula	Not applicable	
Chemical structure ^a	Not applicable	
Identification numbers:		Windholz 1983
CAS registry	8021-39-4	Merck 1989
NIOSH RTECS	G05870000	HSDB 2000
EPA hazardous waste	U051	HSDB 2000
OHM/TADS	No data	
DOT/UN/NA/IMCO	UN 2810; IMO 6.1	HSDB 2000
HSDB	1979	HSDB 2000

^aWood creosote is a mixture composed primarily of phenolic compounds.

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 Substance Data Bank; 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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Chemical Identity of Coal Tar Creosote

Characteristic	Information	Reference
Chemical name	Coal tar creosote	American Wood Preserver's Association 1988
Synonym(s)	Creosote, creosote oil, dead oil, brick oil, coal tar oil, creosote P1, heavy oil, liquid pitch oil, wash oil, creosotum, cresylic creosote, naphthalene oil, tar oil, AWPA #1, Preserv-o-sote	HSDB 2000
Registered trade name(s)	Sakresote 100	HSDB 2000
Chemical formula	Not applicable	
Chemical structure ^a	Not applicable	
Identification numbers:		
CAS registry	8001-58-9	Merck 1989; Weiss 1986
NIOSH RTECS	GF9615000	HSDB 2000
EPA hazardous waste	U051	HSDB 2000
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	UN 1136/1137; IMO 3.2/3.3	HSDB 2000
HSDB	6299	HSDB 2000
NCI	No data	

^aCoal tar creosote is a mixed compound composed primarily of polycyclic aromatic hydrocarbons including phenanthrene, acenaphthene, fluorene, anthracene, and pyridine.

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 Substance 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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-3. Chemical Identity of Coal Tar

Characteristic	Information	Reference
Chemical name	Coal tar	Merck 1989
Synonym(s)	Crude coal tar, pixalbol, tar	HSDB 2000
Registered trade name(s)	Psorigel, Clinitar	Merck 1989
Chemical formula	Not applicable	
Chemical structure ^a	Not applicable	
Identification numbers:		
CAS registry	8007-45-2	HSDB 2000
NIOSH RTECS	No data	
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO	UN 1999; IMO 3.2/3.3	HSDB 2000
HSDB	5050	HSDB 2000
NCI	No data	

^aCoal tar is a mixed compound composed primarily of polycyclic aromatic hydrocarbons including phenanthrene, acenaphthene, fluorene, anthracene, and pyridine.

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 Substance 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

4. CHEMICAL AND PHYSICAL INFORMATION

(guaiacol and 4-methylguaiacol) comprise the bulk of beechwood creosote. Xylenols, other methylated guaiacols, and trimethylphenols account for virtually all of the remaining phenolics in the material. Since beechwood creosote is obtained from different sources using nonstandardized procedures, its composition may vary to some degree. For the sample analyzed by Ogata and Baba (1989), more than two-thirds of the more than 20 compounds identified (Table 4-4) were represented by just four components (phenol, p-cresol, guaiacol, and 4-methylguaiacol). Selected chemical and physical properties of wood creosote are shown in Table 4-5.

Creosote bush resin consists of phenolics (e.g., flavonoids and nordihydroguaiaretic acid), neutrals (e.g., waxes), basics (e.g., alkaloids), and acidics (e.g., phenolic acids). The phenolic portion comprises 83–91% of the total resin. Nordihydroguaiaretic acid accounts for 5–10% of the dry weight of the leaves (Leonforte 1986). No other relevant chemical/physical data are available for creosote bush resin; the substance is therefore not addressed further in this profile.

4.2.2 Coal Tar Creosote, Coal Tar, and Coal Tar Pitch

These three substances are very similar mixtures obtained from the distillation of coal tars. The physical and chemical properties of each are similar, although limited data are available for coal tar, and coal tar pitch. Chemical Abstracts Service Numbers (CAS #) are associated with coal tar creosote (8001-58-9), coal tar pitch (67996-93-2), and coal tar (8007-45-2). Literature searches for coal tar pitch produce data identical to that obtained for coal tar creosote. A distinction between these materials is provided in the following discussion.

Coal tars are by-products of the carbonization of coal to produce coke and/or natural gas. Physically, they are usually viscous liquids or semi-solids that are black or dark brown with a naphthalene-like odor. The coal tars are complex combinations of polycyclic aromatic hydrocarbons, phenols, heterocyclic oxygen, sulfur, and nitrogen compounds. By comparison, coal tar creosotes are distillation products of coal tar. They have an oily liquid consistency and range in color from yellowish-dark green to brown. The coal tar creosotes consist of aromatic hydrocarbons, anthracene, naphthalene, and phenanthrene derivatives. At least 75% of the coal tar creosote mixture is polycyclic aromatic hydrocarbons (PAHs). Unlike the coal tars and coal tar creosotes, coal tar pitch is a residue produced during the distillation of coal tar. The pitch is a shiny, dark brown to black residue which contains polycyclic aromatic hydrocarbons and their methyl and polymethyl derivatives, as well as heteronuclear compounds

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-4. Identity of Major Components of Wood Creosote^a

Compound	Relative peak area, (percent total peak area)
phenol	14.45
methylhydroxycyclopentenone	0.23
o-cresol	3.22
dimethylhydroxycyclopentenone	0.50
p-cresol	13.60
guaiacol	23.76
2,6-xylenol	1.04
3,4-xylenol	0.70
6-methylguaiacol	0.31
3,5-xylenol	2.94
2,4-xylenol	2.80
2,5-xylenol	0.68
unknown	1.31
2,3-xylenol	0.70
3-methylguaiacol	1.85
5-methylguaiacol	1.29
4-methylguaiacol	19.01
2,4,6-trimethylphenol	0.40
2,3,6-trimethylphenol	0.48
4-ethylguaiacol	6.36
4-ethyl-5-methylguaiacol	0.21
4-propylguaiacol	0.45

^aAs identified by gas chromatography/mass spectrometry (Ogata and Baba 1989); composition of wood creosotes may vary from source to source.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-5. Physical and Chemical Properties of Wood Creosote

Property	Information	Reference
Molecular weight	Not applicable	
Color	Yellowish to colorless	Merck 1989
Physical state	Liquid	Weiss 1986
Melting point	No data	
Boiling point	. 203 EC	Merck 1989
Specific gravity at 25 EC	1.08	Merck 1989
Odor	Characteristic smokey odor	Merck 1989
Taste	Caustic, burning taste	Merck 1989
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water	150–200 parts	Merck 1989
Organic solvent(s)	Miscible with alcohol, ether, fixed, or volatile oils	Merck 1989
Partition coefficients:	No data	
Vapor pressure	No data	
Henry's law constant	No data	
Autoignition temperature	No data	
Flashpoint	74 EC (closed cup)	Clayton and Clayton 1981
Flammability limits in air	No data	
Explosive limits	No data	
Other	The major components of wood creosote (phenols) are susceptible to oxidative degradation when exposed to air (oxygen), particularly if the material is basic (high pH).	Not applicable

4. CHEMICAL AND PHYSICAL INFORMATION

(American Wood Preserver's Association 1988). Coal tar creosote is defined by the latter organization as:

A distillate derived from coal tar. As used in the wood preserving industry, creosote denotes a distillate of coal tar produced by the high temperature carbonization of bituminous coal. Coal tar creosote consists principally of liquid and solid aromatic hydrocarbons and contains some tar acids and tar bases; it is heavier than water and has a continuous boiling range beginning at about 200 EC.

Coal tar creosote is now commonly defined by function, and refers to "the fractions or blends of fractions specifically used for timber preservation" (IARC 1987). Coal tar creosote is referred to as "creosote" by the U.S. EPA. The substance is a complex mixture typically composed of approximately 85% PAHs and 2–17% phenolics (Bedient et al. 1984). The composition of the mixture may also vary across lots and across manufacturers. Properties of coal tar creosote are shown in Table 4-6.

Coal tar pitch is the tar distillation residue produced during coking operations (NIOSH 1977). The grade of pitch thus produced is dependent on distillation conditions, including time and temperature. The fraction consists primarily of condensed ring aromatics, including 2–6 ring systems, with minor amounts of phenolic compounds and aromatic nitrogen bases. The number of constituents in coal tar pitch is estimated to be in the thousands (HSDB 2000). A list of the components comprising the PAH fraction of coal tar pitch is shown in Table 4-7. Properties for this substance are similar or identical to those shown in Table 4-6 for coal tar creosote.

Coal tar itself is produced by the carbonization, or coking of coal. Coal tar is defined by Hawley (1977) as:

A black, viscous liquid (or semi-solid), naphthalene-like odor, sharp burning taste; obtained by the destructive distillation of bituminous coal, as in coke ovens; 1 ton of coal yields 8.8 gallons of coal tar. Combustible. Specific gravity 1.18–1.23 (66/60 EF). Soluble in ether, benzene, carbon disulfide, chloroform; partially soluble in alcohol, acetone, methanol, and benzene; only slightly soluble in water.

The composition of the creosote mixture is dependent on the sources and preparation parameters of the coal tar, and as a result the creosote components are rarely consistent in their type and concentration. An example of the composition variability among creosote samples was recently presented by Weyand et al. (1991). In that study, the concentrations of several PAHs were analyzed in four coal tars. All of the PAHs identified exhibited 2-fold to nearly 20-fold differences in concentration among the four samples.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-6. Physical and Chemical Properties of Coal Tar Creosote

Property	Information	Reference
Molecular weight	Not applicable	
Color	Translucent brown to black; oily liquid; yellowish to dark green-brown	Merck 1989
Physical state	Liquid	Weiss 1986
Melting point	No data	
Boiling point	194–400 EC	Clayton and Clayton 1981
Specific gravity	1.07–1.08	Clayton and Clayton 1981
Odor	Aromatic smokey smell Characteristic sharp odor	DOT 1985 Merck 1989
Odor threshold:		
Water	No data	
Air	No data	
Taste	Burning, caustic taste	Clayton and Clayton 1981
Solubility:		
Water	Slightly soluble	Clayton and Clayton 1981
Organic solvent(s)	Miscible with alcohol, ether, fixed or volatile oils	Clayton and Clayton 1981
Partition coefficients:	1.0 (log K_{ow})	HSDB 2000
Vapor pressure	No data	
Autoignition temperature	335 EC	Merck 1996
Flashpoint	74 EC	Merck 1989
Flammability limits in air	No data	
Explosive limits	No data	

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-7. Identity of PAH Components of Coal Tar Pitch^a

Peak No.	Compound ^b	Peak No.	Compound ^b
1	naphthalene	31	acridine
2	benzo(b)thiophene	32	phenanthridine
3	quinoline	33	carbazole
4	2-methylnaphthalene	34	methylphenanthrene, -anthracene
5	1-methylnaphthalene	35	methylphenanthrene, -anthracene
6	biphenyl	36	methylphenanthrene, -anthracene
7	2-ethylnaphthalene	37	4H-cyclopenta(def)phenanthrene
8	dimethylnaphthalene	38	methylphenanthrene, -anthracene
9	dimethylnaphthalene	39	methylphenanthrene, -anthracene
10	dimethylnaphthalene	40	methylcarbazole
11	methylbiphenyl	41	methylcarbazole
12	acenaphthene	42	2-phenylnaphthalene
13	naphthonitrile or azaacenaphthylene	43	dihdropyrene or isomer
14	dibenzofuran	44	fluoranthene
15	fluorene	45	azafluoranthene, -pyrene
16	methylacenaphthene	46	phenanthro(4,5-bcd)thiophene
17	methylacenaphthene	47	azafluoranthene, -pyrene
18	methylacenaphthene	48	pyrene
19	methyldibenzofuran	49	benzonaphthofuran
20	methyldibenzofuran	50	benzacenaphthene or isomer
21	9,10-dihydroanthracene	51	benzacenaphthene or isomer
22	9,10-dihydrophenanthrene	52	benzonaphthofuran
23	methylfluorene	53	benzonaphthofuran
24	methylfluorene	54	benzo(lmn)phenanthridine
25	methylfluorene	55	benzo(kl)xanthene
26	methylfluorene	56	methylfluoranthene, -pyrene
27	1,2,3,4-tetrahydroanthracene	57	4H-benzo(def)carbazole
28	dibenzo(bd)thiophene	58	azafluoranthene, -pyrene
29	phenanthrene	59	benzo(a)fluorene
30	anthracene	60	methylfluoranthene, -pyrene

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-7. Identity of PAH Components of Coal Tar Pitch^a (continued)

Peak No.	Compound ^b	Peak No.	Compound ^b
61	benzo(a)fluorene	91	7H-benzo(c)carbazole
62	benzo(c)fluorene or isomer	92	methylbenz(a)anthracene or isomer
63	methylbenzacenaphthene or isomer	93	tetramethylfluoranthene or isomer
64	methylbenzonaphthofuran or isomer	94	5H-benzo(b)carbazole
65	methylpyrene or isomer	95	methylbenzophenanthridine or isomer
66	methylpyrene or isomer	96	dimethylbenzo(cdf)carbazole
67	methylbenzonaphthofuran or isomer	97	methylchrysene or isomer
68	methylbenzonaphthofuran or isomer	98	methylchrysene or isomer
69	methylazapyrene or isomer	99	methylbenz(a)anthracene or isomer
70	methylbenzonaphthofuran or isomer	100	dimethylbenz(a)anthracene or isomer
71	methylbenzofluorene	101	methylbenz(a)anthracene or isomer
72	dihydrochrysene or isomer	102	dimethylbenz(a)anthracene or isomer
73	dimethylfluoranthene, -pyrene	103	11H-benz(bc)aceanthrylene or isomer
74	trimethylfluoranthene, -pyrene	104	methylbenz(a)anthracene or isomer
75	dimethylfluoranthene, -pyrene	105	4H-cyclopenta(def)chrysene or isomer
76	benzo(b)naphtho(2,1-d)thiophene	106	methylbenz(a)anthracene or isomer
77	benzo(c)phenanthrene	107	binaphthalene or isomer
78	benzo(ghi)fluoranthene	108	4H-cyclopenta(def)triphenylene or isomer
79	dimethylbenzonaphthofuran	109	dimethylbenz(a)anthracene or isomer
80	benzo(b)naphtho(1,2-d)thiophene	110	methylbenz(a)anthracene or isomer
81	dibenzoquinoline or isomer	111	binaphthalene or isomer
82	tetrahydrochrysene or isomer	112	dimethylbenz(a)anthracene or isomer
83	benzo(a)naphtho(2,3-d)thiophene	113	methylbenz(a)anthracene or isomer
84	benz(a)anthracene	114	binaphthalene or isomer
85	chrysene	115	phenylphenanthrene or isomer
86	11H-benzo(a)carbazole	116	dihydrobenzofluoranthene or isomer
87	naphthacene	117	dimethylchrysene or isomer
88	methylbenzonaphthothiophene	118	dibenzophenanthridine or isomer
89	methylbenz(a)anthracene or isomer	119	biquinoline
90	tetramethylfluoranthene or isomer	120	biquinoline

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-7. Identity of PAH Components of Coal Tar Pitch^a (continued)

Peak No.	Compound ^b	Peak No.	Compound ^b
121	benzo(j)fluoranthene	151	methylbenzopyrene or isomer
122	dihydrobenzofluoranthene or isomer	152	methylbenzopyrene or isomer
123	benzo(b)fluoranthene	153	11H-cyclopenta(ghi)perylene or isomer
124	dihydrobenzofluoranthene or isomer	154	methylbenzopyrene or isomer
125	benzo(k)fluoranthene	155	dimethylbenzopyrene or isomer
126	dibenzonaphthofuran or isomer	156	methylbenzopyrene or isomer
127	dihydrobenzofluoranthene or isomer	157	methylbenzopyrene or isomer
128	dimethylchrysene or isomer	158	dimethylbenzopyrene or isomer
129	azabenzopyrene or isomer	159	11H-indeno(2,1,7-cde)pyrene or isomer
130	dibenzonaphthofuran or isomer	160	dimethylbenzopyrene or isomer
131	benzophenanthrothiophene	161	dinaphthothiophene
132	azabenzopyrene or isomer	162	dimethylbenzopyrene or isomer
133	benzo(e)pyrene	163	dibenzophenanthridine or isomer
134	dibenzonaphthofuran or isomer	164	dibenzonaphthothiophene
135	benzo(a)pyrene	165	dimethylbenzopyrene or isomer
136	dibenzonaphthofuran or isomer	166	dibenzocarbazole
137	perylene	167	dimethylbenzopyrene or isomer
138	dibenzonaphthofuran or isomer	168	dibenzo(bg)phenanthrene or isomer
139	methylbenzofluoranthene or isomer	169	benzo(g)chrysene or isomer
140	methylbenzofluoranthene or isomer	170	dinaphthothiophene
141	azabenzopyrene or isomer	171	dimethylbenzofluoranthene or isomer
142	4H-naphtho(1,2,3,4-def)carbazole or isomer	172	dibenzoacridine or isomer
143	methylbenzofluoranthene or isomer	173	dinaphthothiophene
144	dibenzofluorene or isomer	174	dinaphthothiophene
145	dihydroindenopyrene or isomer	175	benzo(c)chrysene or isomer
146	dibenzofluorene or isomer	176	dibenzocarbazole
147	dibenzofluorene or isomer	177	dimethylbenzofluoranthene or isomer
148	methylbenzopyrene or isomer	178	dibenz(aj)anthracene
149	dibenzo(cg)phenanthrene or isomer	179	indenopyrene or isomer
150	dimethyldibenzonaphthofuran or isomer	180	dimethyldibenzonaphthofuran

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-7. Identity of PAH Components of Coal Tar Pitch^a (continued)

Peak No.	Compound ^b	Peak No.	Compound ^b
181	methyl dibenzophenanthrene, -anthracene	191	dimethyl dibenzonaphthofuran
182	indenopyrene or isomer	192	picene
183	methyl benzophenanthrothiophene	193	dimethyl benzopyrene or isomer
184	dibenz(ac)anthracene	194	dimethyl dibenzonaphthofuran
185	methyl dibenzophenanthrene, -anthracene	195	benzo(ghi)perylene
186	dimethyl benzofluoranthene or isomer	196	benzo(a)naphthacene or pentacene
187	dibenz(ah)anthracene	197	dimethyl dibenzonaphthofuran
188	trimethyl benzofluoranthene or isomer	198	anthanthrene
189	dimethyl dibenzophenanthrene, -anthracene	199	methyl indenopyrene or isomer
190	benzo(b)chrysene		

^aAs reported by Guillén et al. 1992; compounds presented in elution order

^bTentative identification by gas chromatography/mass spectrometry

4. CHEMICAL AND PHYSICAL INFORMATION

Benzo[a]pyrene, a component whose individual toxicity has been examined extensively, ranged from nondetectable levels (detection limit 0.3 g/kg) to 1.7, 6.4, and 3.9 g/kg of coal tar.

Limited chemical/physical data exist for coal tar. Table 4-8 summarizes the current information. Because of the variability in feedstock and manufacturing processes, presentation of exact values for various properties presented in Tables 4-6 and 4-8 is not possible.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-8. Physical and Chemical Properties of Coal Tar

Property	Information	Reference
Molecular weight	Not applicable	
Color	Almost black, thick liquid, or semisolid	Merck 1989
Physical state	Semisolid	Weiss 1986
Melting point	No data	
Boiling point	No data	
Specific gravity	1.18–1.23	Hawley 1981
Odor	Naphthalene-like	Osol 1980
Odor threshold:		
Water	No data	
Air	No data	
Taste	Sharp, burning taste	Osol 1980
Solubility:		
Water	Slightly soluble	Merck 1989
Organic solvent(s)	Mostly dissolves in benzene; partially dissolves in alcohol, ether, chloroform, acetone, and petroleum ether	Merck 1989
Partition coefficients	No data	
Vapor pressure	No data	
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Explosive limits	No data	