CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity, chemical synonyms, and identification numbers for wood creosote, coal tar creosote, and coal tar is provided 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. The partitioning behavior of PAHs and other semi-volatile substances between the vapor and particulate phase in air is well understood (Eisenreich et al. 1981; Xie et al. 2014). In general, several of the low molecular weight constituents are semi-volatile and exist in air in the vapor-phase, while larger PAHs are less volatile and tend to exist in the particulate phase; this affects atmospheric transport, degradation, and deposition into the lungs (Volkens and Leith 2003).

Table 4-1. Chemical Identity of Wood Creosote

Characteristic	Information	Reference
Chemical mixture name	Wood creosote	Budavari 1989
Synonym(s) and registered trade name(s)	Beechwood creosote; creosote; creasote	Budavari 1989
Chemical formula[a]	Not applicable	
Chemical structure[a]	Not applicable	
CAS Registry Number	8021-39-4	Budavari 1989
TSCA definition	A complex combination of phenols obtained as a distillate from wood tar.	EPA 2022a

[a]Wood creosote is a mixture composed primarily of phenolic compounds.

CAS = Chemical Abstracts Service; TSCA = Toxic Substances Control Act

Table 4-2. Chemical Identity of Coal Tar Creosote

Characteristic	Information	Reference
Chemical mixture name	Coal tar creosote	AWPA 1988
Synonym(s) and registered trade name(s)	Creosote; standard creosote oil; creosote, coal tar; creosotum; naphthalene oil; heavy oil; brick oil; wash oil; cresylic creosote; coal tar oil; liquid patch oil; petroleum creosote, creosote P1; sakresote 100; Emulsified Refined Coal-Tar (Ready to Use, Commercial Grade; Road Tar (RT-1, RT-2, RT-3, RT-4, RT-5, RT-6, RT-7, RT-8, RT-9, RT-10, RT-11, RT-12, RT.C.B.-5, and RT.C.B.-6)	ASTM 2016, 2017; NLM 2022a
Chemical formula[a]	Not applicable	
Chemical structure[a]	Not applicable	
CAS Registry Number	8001-58-9	Budavari 1989; Weiss 1986; NLM 2022a
TSCA definition	The distillate of coal tar produced by the high temperature carbonization of bituminous coal. It consists primarily of aromatic hydrocarbons, tar acids, and tar bases.	EPA 2022a

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

CAS = Chemical Abstracts Service; TSCA = Toxic Substances Control Act

Table 4-3. Chemical Identity of Coal Tar

Characteristic	Information	Reference
Chemical mixture name	Coal tar	Budavari 1989
Synonym(s) and registered trade name(s)	Crude coal tar; pixalbol; tar; Psorigel; Clinitar; coal tar extract	Budavari 1989; NLM 2022b
Chemical formula[a]	Not applicable	
Chemical structure[a]	Not applicable	
CAS Registry Number	8007-45-2	NLM 2022b
TSCA definition	The byproduct from the destructive distillation of coal. Almost black semisolid. A complex combination of aromatic hydrocarbons, phenolic compounds, nitrogen bases, and thiophene.	EPA 2022a

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

CAS = Chemical Abstracts Service; TSCA = Toxic Substances Control Act

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.

Wood Creosote. Wood creosotes are derived from either beechwood (referred to herein as beechwood creosote) or 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 stimulating expectorant, but it is not a major pharmaceutical ingredient today in the United States. Beechwood creosote is obtained from fractional distillation (200–220°C at atmospheric pressure) of beechwood or related plants. The mixture has been characterized by Ogata and Baba (1989). Phenol, *p*-cresol, and guaiacols (guaiacol and 4-methylguaiacol) comprise the bulk of beechwood creosote. Xylenols, other methylated guaiacols, and trimethylphenols account for virtually all 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 (see 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.

Table 4-4. Identity of Major Components of Beechwood Creosote[a]

Compound	Relative peak area (percentage identified in mixture)
Phenol	14.5%
Methylhydroxycyclopentenone	0.23%
o-Cresol	3.22%
Dimethylhydroxycyclopentanone	0.50%
p-Cresol	13.6%
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%

Table 4-4. Identity of Major Components of Beechwood Creosote[a]

Compound	Relative peak area (percentage identified in mixture)
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%

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

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

Property	Information	Reference
Molecular weight	Not applicable	
Color	Yellowish to colorless	Budavari 1989
Physical state	Liquid	Weiss 1986
Melting point	No data	
Boiling point	203°C	Budavari 1989
Density at 20°C	Not applicable	
Odor	Characteristic smokey odor	Budavari 1989
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water	150–200 parts water	Budavari 1989
Organic solvents	Miscible with alcohol, ether, fixed or volatile oils	Budavari 1989
Partition coefficients:		
Log K_{ow}	Not applicable	
Log K_{oc}	Not applicable	
Vapor pressure at 20°C	Not applicable	
Henry's law constant at 25°C	Not applicable	
Autoignition temperature	No data	
Flashpoint	74°C (closed cup)	Clayton and Clayton 1981
Flammability limits	No data	
Conversion factors	Not applicable	

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

Explosive limits	No data

[a]Physical-chemical properties will vary by sample as the constituents of the complex mixture are not constant. Not applicable has been used for several properties since a wide range of values are expected based upon chemical composition of the mixture.

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.

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 (CAS) Registry Numbers 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 byproducts 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 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 (AWPA 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°C (AWPA 1988).

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). The substance is a complex mixture typically composed of approximately 85% PAHs and 2–17% phenolics (Bedient et al. 1984). 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 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. 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.

The International Programme on Chemical Safety (IPCS) Concise International Chemical Assessment Document (CICAD) for coal tar creosote lists some common constituents of some coal tar creosotes that were analyzed for their chemical identity (IPCS 2004). These are summarized in Table 4-6.

Table 4-6. Some Constituents and Weight Percentage of Eight Coal Tar Creosote Mixtures

	Weight percentage[a]							
Coal tar creosote mixture A		B	C	D	E	F	G	H
Aromatic hydrocarbons								
Indene					0.6	0.43	0.87	
Biphenyl	0.8/1.6	2.1	1–4	0.8	1.3	1.45	4.1	
PAHs								
Naphthalene	1.3/3.0*	11	13–18	7.6	12.9	12.32	11.4	
1-Methylnaphthalene	0.9*/1.7		12–17	0.9	2.2	3.29	8.87	
2-Methylnaphthalene	1.2*/2.8	3.0	12.0	2.1	4.5	7.51	11.5	
Dimethylnaphthalenes	2.0*/2.3	5.6			1.6	3.42	5.16	
Acenaphthylene					0.2	0.15	0.1	
Acenaphthene	9.0*/14.7	3.1	9.0	8.3	5.8	12.51	5.86	
Fluorene	7.3/10.0*	3.1	7–9	5.2	4.6	5.03	6.33	
Methylfluorenes	2.3/3.0*				3.1			
Phenanthrene	21*	12.2	12–16	16.9	11.2	10.21	6.7	1–3.3
Methylphenanthrenes	3.0*				3.1	0.45	0.54	
Anthracene	2.0*		2–7	8.2	1.7	0.9	0.8	0.4–1.2
Methylanthracenes	4.0*	5.9						

Table 4-6. Some Constituents and Weight Percentage of Eight Coal Tar Creosote Mixtures

	Weight percentage[a]							
Coal tar creosote mixture	A	B	C	D	E	F	G	H
Fluoranthene	7.6/10.0*	3.4	2–3	7.5	4.6	4.41	2.27	0.2–2.2
Pyrene	7.0/8.5*	2.2	1–5	5.3	3.7	2.0	1.13	0.1–1.5
Benzofluorenes	1.0/2.0*	3.4			2.2			
Benz[a]anthracene					0.5	0.26	0.17	
Benzo[k]fluoranthene					0.22			0.16–0.3
Chrysene	2.6/3.0*	2.2	1		0.5–1.0	0.21	<0.05	
Benzo[a]pyrene				0.43	0.2	<0.1	<0.05	0.02–0.16
Benzo[e]pyrene					0.2			
Perylene					0.1			
Tar acids/phenolics								
Phenol					0.24	0.56	0.24	
o-Cresol					0.10		0.2	
m-, *p*-Cresol					0.24	2.31	0.6	
2,4-Dimethylphenol					0.12	0.59	0.48	
Naphthols					0.12			
Tar bases/nitrogen-containing heterocycles								
Indole				2				
Quinoline			1	2.0	0.59	0.58	0.89	
Isoquinoline				0.7	0.18	0.30	0.59	
Benzoquinoline				4	0.29	0.05	0.5	
Methylbenzoquinoline				0.3				
Carbazole		2.4		3.9	0.7	0.53	0.22	
Methylcarbazoles				2				
Benzocarbazoles				2.8	0.1			
Dibenzocarbazoles				3.1				
Acridine				2	0.2	1.5	0.12	
Aromatic amines								
Aniline				0.05	0.21			
Sulfur heterocycles								
Benzothiophene				0.3	0.4	0.3	0.5	
Dibenzothiophene					1.0	0.78	0.73	
Oxygen-containing heterocycles/furans								
Benzofuran						<0.1	<0.1	
Dibenzofuran	5.0*/7.5	1.1	4–6	3.9	3.7	6.14	5.59	

Table 4-6. Some Constituents and Weight Percentage of Eight Coal Tar Creosote Mixtures

	Weight percentage[a]						
Coal tar creosote mixture A	B	C	D	E	F	G	H
Other not specified components							
Unidentified component				23.1			

[a]An asterisk indicates that data were obtained from a literature survey; measurements without an asterisk indicate main components in an AWPA standard creosote.

AWPA = American Wood-Preservers' Association; PAH = polycyclic aromatic hydrocarbon

Source: IPCS 2004

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°F). Soluble in ether, benzene, carbon disulfide, chloroform; partially soluble in alcohol, acetone, methanol, and benzene; only slightly soluble in water.

The composition of the mixture will vary across lots and across manufacturers. Gallacher et al. (2017a, 2017b) performed an analysis of 16 coal tar samples obtained from five different production processes. They identified a total of 2,369 unique compounds. This included 948 aromatics, 196 aliphatics, 380 sulfur-containing compounds, 209 oxygen-containing compounds, 262 nitrogen-containing compounds, and 865 heterocyclic compounds (15 mixed heterocycles); of all the PAHs, 359 were hydroxylated. The contents of both heterocyclic and hydroxylated PAHs varied greatly with the production process used. Of the 2,369 compounds identified, 173 were found to be present in all samples (the majority of these were PAHs). A full list of these compounds can be obtained (Gallacher et al. (2017c). Properties of coal tar creosote are shown in Table 4-7.

Table 4-7. Physical and Chemical Properties of Coal Tar Creosote[a]

Property	Information	Reference
Molecular weight	Not applicable[b]	
Color	Translucent brown to black; oily liquid; yellowish to dark green-brown	Budavari 1989
Physical state	Liquid	Weiss 1986
Melting point	No data	

Table 4-7. Physical and Chemical Properties of Coal Tar Creosote[a]

Boiling point	194–400°C	Clayton and Clayton 1981
Density at 20°C	Not applicable	
Odor	Aromatic smokey smell; characteristic smokey odor	Budavari 1989; DOT 1985
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water	Slightly soluble	Clayton and Clayton 1981
Organic solvents	Miscible with alcohol, ether, fixed or volatile oils	Clayton and Clayton 1981
Partition coefficients:		
Log K_{ow}	Not applicable	
Log K_{oc}	Not applicable	
Vapor pressure at 20°C	Not applicable	
Henry's law constant at 25°C	Not applicable	
Autoignition temperature	335°C	Budavari 1989
Flashpoint	74°C (closed cup)	Budavari 1989
Flammability limits	No data	
Conversion factors	Not applicable	
Explosive limits	No data	

[a]Physical-chemical properties will vary by sample as the constituents of the complex mixture are not constant.
[b]Not applicable has been used for several properties since a wide range of values are expected based upon chemical composition of the mixture.

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 (EPA 2015). A list of the components comprising the PAH fraction of coal tar pitch is shown in Table 4-8. Table 4-9 summarizes physical/chemical data for coal tar. Properties for this substance are similar or identical to those shown in Table 4-7 for coal tar creosote. Because these substances are all complex mixtures, physical-chemical properties such as log K_{ow} and Henry's Law constants cannot be represented by a single value. Ranges of values for several physical-chemical properties for the chemical classes of coal tar creosote have been published (IPCS 2004). Because of the variability in feedstock and manufacturing processes, presentation of exact values for various properties presented in Tables 4-7 and 4-9 is not possible.

Table 4-8. Identity of PAH Components of Coal Tar Pitch[a]

Peak No.	Compound[b]	Peak No.	Compound[b]
1	Naphthalene	101	Methylbenz[a]anthracene or isomer
2	Benzo[b]thiophene	102	Dimethylbenz[a]anthracene or isomer
3	Quinoline	103	11H-Benz[bc]aceanthrylene or isomer
4	2-Methylnaphthalene	104	Methylbenz[a]anthracene or isomer
5	1-Methylnaphthalene	105	4H-Cyclopenta[def]chrysene or isomer
6	Biphenyl	106	Methylbenz[a]anthracene or isomer
7	2-Ethylnaphthalene	107	Binaphthalene or isomer
8	Dimethylnaphthalene	108	4H-Cyclopenta[def]triphenylene or isomer
9	Dimethylnaphthalene	109	Dimethylbenz[a]anthracene or isomer
10	Dimethylnaphthalene	110	Methylbenz[a]anthracene or isomer
11	Methylbiphenyl	111	Binaphthalene or isomer
12	Acenaphthene	112	Dimethylbenz[a]anthracene or isomer
13	Naphthonitrile or azaacenaphthylene	113	Methylbenz[a]anthracene or isomer
14	Dibenzofuran	114	Binaphthalene or isomer
15	Fluorene	115	Phenylphenanthrene or isomer
16	Methylacenaphthene	116	Dihydrobenzofluoranthene or isomer
17	Methylacenaphthene	117	Dimethylchrysene or isomer
18	Methylacenaphthene	118	Dibenzophenanthridine or isomer
19	Methyldibenzofuran	119	Biquinoline
20	Methyldibenzofuran	120	Biquinoline
21	9,10-Dihydroanthracene	121	Benzo[j]fluoranthene
22	9,10-Dihydrophenanthrene	122	Dihydrobenzofluoranthene or isomer
23	Methylfluorene	123	Benzo[b]fluoranthene
24	Methylfluorene	124	Dihydrobenzofluoranthene or isomer
25	Methylfluorene	125	Benzo[k]fluoranthene
26	Methylfluorene	126	Dibenzonaphthofuran or isomer
27	1,2,3,4-Tetrahydroanthracene	127	Dihydrobenzofluoranthene or isomer
28	Dibenzo[bd]thiophene	128	Dimethylchrysene or isomer
29	Phenanthrene	129	Azabenzopyrene or isomer
30	Anthracene	130	Dibenzonaphthofuran or isomer
31	Acridine	131	Benzophenanthrothiophene
32	Phenanthridine	132	Azabenzopyrene or isomer
33	Carbazole	133	Benzo[e]pyrene
34	Methylphenanthrene, -anthracene	134	Dibenzonaphthofuran or isomer
35	Methylphenanthrene, -anthracene	135	Benzo[a]pyrene
36	Methylphenanthrene, -anthracene	136	Dibenzonaphthofuran or isomer
37	4H-Cyclopenta[def]phenanthrene	137	Perylene
38	Methylphenanthrene, -anthracene	138	Dibenzonaphthofuran or isomer
39	Methylphenanthrene, -anthracene	139	Methylbenzofluoranthene or isomer
40	Methylcarbazole	140	Methylbenzofluoranthene or isomer
41	Methylcarbazole	141	Azabenzopyrene or isomer

Table 4-8. Identity of PAH Components of Coal Tar Pitch[a]

Peak No.	Compound[b]	Peak No.	Compound[b]
42	2-Phenylnaphthalene	142	4H-Naphtho[1,2,3,4-def]carbazole or isomer
43	Dihydropyrene or isomer	143	Methylbenzofluoranthene or isomer
44	Fluoranthene	144	Dibenzofluorene or isomer
45	Azafluoranthene, -pyrene	145	Dihydroindenopyrene or isomer
46	Phenanthro[4,5-bcd]thiophene	146	Dibenzofluorene or isomer
47	Azafluoranthene, -pyrene	147	Dibenzofluorene or isomer
48	Pyrene	148	Methylbenzopyrene or isomer
49	Benzonaphthofuran	149	Dibenzo[cg]phenanthrene or isomer
50	Benzacenaphthene or isomer	150	Dimethyldibenzonaphthofuran or isomer
51	Benzacenaphthene or isomer	151	Methylbenzopyrene or isomer
52	Benzonaphthofuran	152	Methylbenzopyrene or isomer
53	Benzonaphthofuran	153	11H-Cyclopenta[ghi]perylene or isomer
54	Benzo[lmn]phenanthridine	154	Methylbenzopyrene or isomer
55	Benzo[kl]xanthene	155	Dimethylbenzopyrene or isomer
56	Methylfluoranthene, -pyrene	156	Methylbenzopyrene or isomer
57	4H-Benzo[def]carbazole	157	Methylbenzopyrene or isomer
58	Azafluoranthene, -pyrene	158	Dimethylbenzopyrene or isomer
59	Benzo[a]fluorene	159	11H-Indeno[2,1,7-cde]pyrene or isomer
60	Methylfluoranthene, -pyrene	160	Dimethylbenzopyrene or isomer
61	Benzo[a]fluorene	161	Dinaphthothiophene
62	Benzo[c]fluorene or isomer	162	Dimethylbenzopyrene or isomer
63	Methylbenzacenaphthene or isomer	163	Dibenzophenanthridine or isomer
64	Methylbenzonaphthofuran or isomer	164	Dibenzonaphthothiophene
65	Methylpyrene or isomer	165	Dimethylbenzopyrene or isomer
66	Methylpyrene or isomer	166	Dibenzocarbazole
67	Methylbenzonaphthofuran or isomer	167	Dimethylbenzopyrene or isomer
68	Methylbenzonaphthofuran or isomer	168	Dibenzo[bg]phenanthrene or isomer
69	Methylazapyrene or isomer	169	Benzo[g]chrysene or isomer
70	Methylbenzonaphthofuran or isomer	170	Dinaphthothiophene
71	Methylbenzofluorene	171	Dimethylbenzofluoranthene or isomer
72	Dihydrochrysene or isomer	172	Dibenzoacridine or isomer
73	Dimethylfluoranthene, -pyrene	173	Dinaphthothiophene
74	Trimethylfluoranthene, -pyrene	174	Dinaphthothiophene
75	Dimethylfluoranthene, -pyrene	175	Benzo[c]chrysene or isomer
76	Benzo[b]naphtho(2,1-d)thiophene	176	Dibenzocarbazole
77	Benzo[c]phenanthrene	177	Dimethylbenzofluoranthene or isomer
78	Benzo[ghi]fluoranthene	178	Dibenz[aj]anthracene
79	Dimethylbenzonaphthofuran	179	Indenopyrene or isomer
80	Benzo[b]naphtho[1,2-d]thiophene	180	Dimethyldibenzonaphthofuran
81	Dibenzoquinoline or isomer	181	Methyldibenzophenanthrene, anthracene

Table 4-8. Identity of PAH Components of Coal Tar Pitch[a]

Peak No.	Compound[b]	Peak No.	Compound[b]
82	Tetrahydrochrysene or isomer	182	Indenopyrene or isomer
83	Benzo[a]naphtho[2,3-d]thiophene	183	Methylbenzophenanthrothiophene
84	Benz[a]anthracene	184	Dibenz[ac]anthracene
85	Chrysene	185	Methyldibenzophenanthrene, anthracene
86	11H-Benzo[a]carbazole	186	Dimethylbenzofluoranthene or isomer
87	Naphthacene	187	Dibenz[ah]anthracene
88	Methylbenzonaphthothiophene	188	Trimethylbenzofluoranthene or isomer
89	Methylbenz[a]anthracene or isomer	189	Dimethyldibenzophenanthrene, anthracene
90	Tetramethylfluoranthene or isomer	190	Benzo[b]chrysene
91	7H-benzo[c]carbazole	191	Dimethyldibenzonaphthofuran
92	Methylbenz[a]anthracene or isomer	192	Picene
93	Tetramethylfluoranthene or isomer	193	Dimethylbenzopyrene or isomer
94	5H-benzo[b]carbazole	194	Dimethyldibenzonaphthofuran
95	Methylbenzophenanthridine or isomer	195	Benzo[ghi]perylene
96	Dimethylbenzo[cdf]carbazole	196	Benzo[a]naphthacene or pentacene
97	Methylchrysene or isomer	197	Dimethyldibenzonaphthofuran
98	Methylchrysene or isomer	198	Anthanthrene
99	Methylbenz[a]anthracene or isomer	199	Methyl indenopyrene or isomer
100	Dimethylbenz[a]anthracene or isomer		

[a]The amount and specific PAHs in coal tar pitch will vary as the constituents of the complex mixture are not constant.
[b]PAHs identified in GC-MS elution peaks from a coal tar sample. Some PAHs will elute in multiple peaks.

GC-MS = gas chromatography-mass spectrometry; PAH = polycyclic aromatic hydrocarbon

Source: Guillén et al. 1992

Table 4-9. Physical and Chemical Properties of Coal Tar[a]

Property	Information	Reference
Molecular weight	Not applicable[b]	
Color	Almost black, thick liquid, or semisolid	Budavari 1989
Physical state	Semisolid	Weiss 1986
Melting point	No data	
Boiling point	No data	
Density at 20°C	Not applicable	
Odor	Naphthalene-like	Osol 1980
Odor threshold:		
Water	No data	
Air	No data	

Table 4-9. Physical and Chemical Properties of Coal Tar[a]

Solubility:		
Water	Slightly soluble	Budavari 1989
Organic solvents	Mostly dissolves in benzene; partially dissolves in alcohol, ether, chloroform, acetone, and petroleum ether	Budavari 1989
Partition coefficients:		
Log K_{ow}	Not applicable	
Log K_{oc}	Not applicable	
Vapor pressure at 20°C	No data	
Henry's law constant at 25°C	Not applicable	
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Conversion factors	Not applicable	
Explosive limits	No data	

[a]Physical-chemical properties will vary by sample as the constituents of the complex mixture are not constant.
[b]Not applicable has been used for several properties since a wide range of values are expected based upon chemical composition of the mixture.