

The Composition of Cigarette Smoke: A Catalogue of the Polycyclic Aromatic Hydrocarbons*

by

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SUMMARY

Classified as toxicants in many of the substances to which humans are exposed are the polycyclic aromatic hydrocarbons (PAHs). Such exposures include air pollutants from a variety of sources, foodstuffs and beverages, and tobacco smoke. Since the early 1950s, the composition of the latter has been more completely defined than that of any other consumer product. Nearly 4800 components have been identified in tobacco smoke and among these are over 500 PAHs either completely or partially identified. Because of the tumorigenicity of many PAHs, much research has been conducted in attempts to define the relationship between the PAH structures and their specific tumorigenicities in laboratory animals. None of the theories to date completely answers all the questions.

As a prelude to an attempt to develop a more reasonable PAH structure-tumorigenicity relationship, the PAHs completely or partially identified in cigarette smoke have been catalogued. In the catalogue, they are categorized as bicyclic, tricyclic, tetracyclic, etc. with each group subdivided into all-benzenoid PAHs and cyclopentanoid-benzenoid PAHs. Another tabulation includes the PAHs considered in several previous studies on structure-tumorigenicity relationships, studies that dealt primarily with all-benzenoid PAHs. [Beitr. Tabakforsch. Int. 22 (2006) 13–69]

ZUSAMMENFASSUNG

Mit toxisch eingestuften polycyclischen aromatischen Kohlenwasserstoffen (PAHs) sind Menschen vielfach exponiert. Die Expositionen umfassen Luftverschmutzung durch eine Vielzahl von Quellen, Lebensmittel, Getränke und Tabakrauch. Seit den frühen fünfziger Jahren des vorigen Jahrhunderts wurde die Zusammensetzung des

letzteren umfassender untersucht als jedes andere Konsumgut. Fast 4800 Einzelsubstanzen wurden im Tabakrauch nachgewiesen und unter diesen sind mehr als 500 PAHs entweder vollständig oder teilweise identifiziert. Wegen der tumorigenen Wirkung vieler PAHs wurde in vielen Studien versucht, den Zusammenhang zwischen der Struktur der PAHs und ihrer spezifischen tumorigenen Wirkung bei Labortieren zu untersuchen. Durch keine dieser Theorien lassen sich bis heute alle Fragen vollständig beantworten. Als erster Schritt eines Versuchs, eine schlüssigere Beziehung zwischen der Struktur der PAHs und ihrer tumorigenen Wirkung zu entwickeln, wurden die PAHs, die vollständig oder teilweise im Zigarettenrauch identifiziert sind, katalogisiert. In dieser Systematisierung wird unterschieden zwischen bicyclischen, tricyclischen, tetracyclischen usw. PAHs, wobei wiederum jede Gruppe unterteilt ist in benzenoide und cyclopentanoide-benzenoide PAHs. Eine andere Einteilung bezieht sich auf diejenigen PAHs, die Gegenstand mehrerer früherer Studien waren, in denen der Zusammenhang zwischen Struktur und Tumorigenität, hauptsächlich benzenoide PAHs, untersucht wurde. [Beitr. Tabakforsch. Int. 22 (2006) 13–69]

RESUME

Les hydrocarbures polynucléaires aromatiques (PAHs), contenus dans de nombreuses substances auxquelles l'homme est exposé, sont classifiés comme toxiques. Parmi ces expositions comptent les polluants de l'air de sources multiples, l'alimentation, les boissons ou la fumée du tabac. Depuis le début des années 1950, la composition chimique de cette dernière a été analysée de façon plus approfondie que tout autre produit de consommation. Environ 4800 substances ont été identifiées dans la fumée du tabac et parmi celles-ci plus de 500 PAHs complètement ou partiellement identifiées. Due à la tumorigenicité de nombreux

PAHs, beaucoup d'études ont été menées en vue d'examiner la relation entre les structures des PAHs et leurs tumorigénités spécifiques chez les animaux de laboratoire. Jusqu'à présent aucune de ces théories n'explique complètement toutes les questions.

Une approche dans le but de développer une relation plus raisonnable entre la structure et la tumorigénicité des PAHs, est la classification des PAHs complètement ou partiellement identifiés. Dans ce catalogue, les PAHs sont classifiés comme bicycliques, tricycliques, tetracycliques, etc., chaque groupe étant subdivisé en PAHs benzenoid et cyclopentanoid-benzenoid. Un autre catalogue comprend les PAHs examinés dans des études antérieures sur la relation entre la structure et la tumorigénicité, surtout des PAHs benzenoid. [Beitr. Tabakforsch. Int. 22 (2006) 13–69]

INTRODUCTION

Tobacco and tobacco products in the forms of leaf, shredded or grounded tobacco, and various forms of cigars and cigarettes have been available to individuals for ages. For centuries people have enjoyed tobacco but have been admonished of its potential health concerns. Health concerns for cigarette smokers have increased steadily since the early 1950s due to the rapid development and advancement in separation sciences, toxicology and medicine. In his 1954 publication, KOSAK (194) was the first person to catalogue compounds reported in tobacco smoke. His list contained fewer than 100 compounds and a significant number were incorrectly characterized. Today nearly 4800 compounds have been identified as components in tobacco smoke [see Figure 1, p. 140 in (125)]. Over the past fifty years, the Tobacco Industry has made significant progress in both the identification of tobacco and smoke components and the development of technologies to reduce cigarette smoke yields. Significant efforts continue in government, academia, and especially the Tobacco Industry to understand the health effects of smoking and to develop cigarette products with reduced health risks for smokers. One class of tobacco smoke components that has been studied extensively and intensively is the polycyclic aromatic hydrocarbons (PAH) due to their potential health concerns.

Periodically, tobacco researchers have reported the progress on the identification of tobacco and smoke components. Review articles by JOHNSTONE and PLIMMER (182) and IZAWA (177) detailed the tobacco and smoke research conducted over 100 years. IZAWA listed 440 identified smoke components by 1961. QUIN (289) published a review of components found in tobacco and smoke. HERRMANN (151) reviewed phenolic compounds in tobacco smoke. In 1963, PHILIP MORRIS (278) published a monograph on tobacco and smoke composition, a copy of which was provided the Advisory Committee on smoking and health to the US Surgeon General (445). In 1964, ELMENHORST and RECKZEH (97) tabulated the aromatic hydrocarbons identified in tobacco smoke. KUHN (202) published an article on alkaloids in tobacco and smoke. In their 1967 book, WYNDER and HOFFMANN (508) discussed tobacco and smoke chemistry and the results of animal studies with tobacco smoke. ELMENHORST and SCHULTZ (98) listed 250 low-boiling

components and vapor-phase components identified in tobacco smoke. In his 1968 review, STEDMAN (425) listed nearly 1200 identified tobacco and smoke components. The next year, NEURATH (256) reported on the presence of 180 nitrogen-containing compounds in smoke. With the meaningful advancements in analytical methodology, the number of tobacco and smoke components increased dramatically (125). At R. J. Reynolds Tobacco Company (RJRT), SCHUMACHER *et al.* (391), HECKMAN and BEST (147), and NEWELL *et al.* (264) identified over 1500 compounds in the water-soluble and ether-soluble fractions of tobacco smoke. In 1977, SCHMELTZ and HOFFMANN (381) catalogued nearly 500 *N*-containing compounds identified in tobacco smoke but their catalogue did not include the more than 230 *N*-containing compounds newly identified in tobacco smoke by HECKMAN and BEST (147). Between 1974 and 1978, SNOOK *et al.* (416, 419–422) published the results of their massive study of the PAHs identified in tobacco smoke, a study that was followed by an equally definitive one published in 1981 on the azarenes in tobacco smoke (418). In 1980, ISHIGURO and SUGAWARA (176) listed 1889 identified tobacco smoke components in their monograph. However, a tally of the reported tobacco smoke components at that time exceeded 2500. No additional catalogues of the total number of identified components of cigarette mainstream smoke (MSS) have been published since the 1980 ISHIGURO and SUGAWARA (176) publication. SMITH *et al.* (413) recently reported the chemical structures of the 253 identified phenols reported in cigarette MSS.

Numerous catalogues of PAHs identified in MSS have been compiled from 1955 through 2005, including this report. Table 1 is a chronology of catalogues of PAHs in MSS. It contains the year of each catalogue, author (and reference), and the number of PAHs listed. The previous catalogues contain much overlap in terms of the PAHs identified. This report attempts to eliminate the overlap and clearly present the 539 PAHs identified in MSS. Our present report is intended to present a referenced catalogue of the either completely or partially characterized^a PAHs in tobacco smoke. The catalogue contains the chemical name, structure, molecular weight, molecular formula, CAS registration number, and alphabetical listing of references on PAHs.

THE IDENTIFICATION OF POLYCYCLIC AROMATIC HYDROCARBONS IN CIGARETTE MAINSTREAM SMOKE

The significant increase in the number of studies on tobacco smoke composition was triggered by the following events: a) The results in the early 1950s from several retrospective epidemiology studies (487) in which it was reported that an association existed between cigarette smoking and the incidence of lung cancer in smokers, b) a 1953 report of the production of skin carcinoma in susceptible laboratory animals skin painted repeatedly with a concentrated solution of cigarette MSS condensate supposedly produced under conditions simulating the human

^a The term "partially characterized" or "partially identified" indicates that the position of one or more alkyl substituents was not determined.

Table 1. Chronology of catalogues of PAHs in MSS

Year	Author	No. of PAHs listed	Ref.
1954	Kosak	4 ^a	194
1955	Latimer	10	211
1957	Latimer and Rodgman	33	212
1958	Rodgman	36	313
1959	Johnstone and Plimmer	57	182
1960	Rodgman and Menz	68	337
1962	Rodgman <i>et al.</i>	77	339
1963	Philip Morris	61	278
1963	Rodgman <i>et al.</i>	77	340
1964	Elmenhorst and Reckzeh	70	97
1965	Rodgman <i>et al.</i>	85	338
1967	Rodgman and Woosley	85	342
1968	Stedman	79	425
1975	Roberts <i>et al.</i>	206	303
1976	Snook <i>et al.</i>	252 ^b	421
1977	Snook <i>et al.</i>	157 ^b	419
1978	Snook <i>et al.</i>	438 ^b	420
1980	Ishiguro and Sugawara	191	176
1997	Williams <i>et al.</i>	427 ^c	475
2005	Rodgman and Perfetti	539 ^d	current

^a Three of the PAHs listed were identified in a destructive distillate of tobacco, not in tobacco smoke.

^b In the three articles on the PAH study by SNOOK *et al.* (419–421), some identified PAHs were listed in more than one article.

^c In several instances, more than one isomer was reported for some monoalkyl-, dialkyl-, trialkyl-, and tetraalkyl-PAHs but the positions of the alkyl groups were not determined. In the case of such multiple alkyl isomers, only one was listed in this report.

^d This list includes the number of isomers of monoalkyl-, dialkyl-, trialkyl-, and tetraalkyl-PAHs reported where the positions of the alkyl groups were not determined.

smoking of a cigarette (488), c) the realization in 1954 that very little (194) was known about the composition of tobacco smoke to which consumers had been exposed for nearly 400 years, and d) the incorporation of chromatography into the overall methodology of the fractionation of complex mixtures such as tobacco smoke.

Naturally, these findings raised several questions. The first dealt with the identity of the cigarette MSS component(s) responsible for the smoking-lung cancer association in smokers and the skin tumor induction in laboratory animals. Because of extensive data generated on the specific tumorigenicity of about 25% of the hundreds of PAHs synthesized between 1929 and the early 1950s (144), PAHs were considered the most likely tumorigenic agents in cigarette MSS even though their presence was not certain. Eventually, numerous PAHs were identified in cigarette MSS. Because of its MSS level and its high specific tumorigenicity in several bioassays, one PAH was subjected to intense scrutiny: Benzo[*a*]pyrene (B[*a*]P). As a carcinogen, B[*a*]P elicited carcinomas at the painting site in the mouse-skin bioassay. As a sarcogen, B[*a*]P elicited sarcomas in rodent bioassays involving subcutaneous injection.

One class of tobacco smoke components studied extensively is the polycyclic aromatic hydrocarbons. As reported by RODGMAN (323), between 1950 and 1970, an extensive amount of research was conducted on tobacco- and cigarette smoke-related topics. The information generated led to the development of several significant cigarette design

technologies that resulted in the modification of the delivery and composition of cigarette MSS.

The following is a brief chronology of the events occurring in the tobacco smoke-PAH situation: In 1939, the PAHs anthracene, phenanthrene, and B[*a*]P were reported as components of a tobacco-related material by ROFFO (346–349) and his son (345). In discussions of tobacco smoke, the ROFFO findings are generally disregarded because the three PAHs they reported were not detected in tobacco smoke but in a destructive distillate of tobacco. However, ROFFO did report another finding that led to much research both within and outside the Tobacco Industry. ROFFO reported that comparison of the destructive distillate of tobacco with that of an ethanol-extracted tobacco indicated (350) that the PAH content and specific tumorigenicity of the extracted tobacco destructive distillate were reduced from those of the destructive distillate from the control tobacco. ROFFO speculated that the precursors of the tumorigenic PAH components of his distillates were ethanol-soluble phytosterols. Eventually his prediction, as far as it went, was found to be true for cigarette MSS (327, 398). Because he was unaware of the presence in tobacco of long-chained terpenoids such as solanesol, identified in flue-cured tobacco in 1957 by ROWLAND *et al.* (355), ROFFO obviously could not include them in his 1942 precursor prediction. It should be noted that the findings by ROFFO on destructive distillates of tobacco were subsequently equivalent to the effects observed in smoked tobacco, i.e., organic solvent-extraction of a tobacco or tobacco blend which was then incorporated into cigarettes gave MSS with reduced PAH levels and specific tumorigenicity to mouse skin compared to the MSS from control tobacco. However, usually the reduction in specific tumorigenicity was less than the reduction in PAHs, particularly B[*a*]P.

The generation in the early 1950s of carcinomas in laboratory animals (mice) skin-painted with a solution of the mainstream 'tar' from commercial cigarettes (488) led to numerous studies to identify the possible causative agent(s) in the 'tar'. Since much more tumorigenicity data and knowledge were available on PAHs than on any other class of compounds, most of the effort was concentrated on identifying PAHs in cigarette smoke condensate (CSC) as the possible cause of the tumorigenicity. Because of its demonstrated potency as an initiator of carcinomas on skin painting and the wealth of information on it, B[*a*]P became the target of much research on CSC. In 1951, HARTWELL (144) listed nearly 350 studies on the tumorigenicity of B[*a*]P administered in various ways to various species. The other previously studied PAHs were dibenz[*a,h*]anthracene (DB[*a,h*]A) and 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) with 240 and 303 reported biological studies, respectively. Benz[*a*]anthracene (B[*a*]A) and 7,12-dimethylbenz[*a*]anthracene (DMB[*a*]A) were listed with 20 and 32 studies, respectively. In the 20 studies reported by HARTWELL (144), a malignant tumor was noted in only one instance with B[*a*]A.

Although B[*a*]P was reported as a CSC component in the mid-1950s by several American (6, 46–48) and British investigators (69) on the basis of spectral evidence, FIESER, as late as 1957 (104), considered the published evidence to be inadequate as proof of the presence of B[*a*]P in CSC.

Obviously, in 1957 FIESER was unaware of the report by RODGMAN in 1956 (308) on the isolation of crystalline B[a]P from MSS or the reports by FALK and KOTIN in 1955 and 1956 (100) on the determination of the per cigarette yields of B[a]P (plus B[a]A and dibenzo[*def,p*]chrysene) in MSS and sidestream smoke (SSS). Shortly thereafter, in 1959, WYNDER and HOFFMANN reported the isolation of B[a]P in crystalline form from CSC (490), thus ending the controversy about its presence in cigarette smoke.

In 1954, knowledge of cigarette MSS composition was extremely limited. As mentioned earlier, KOSAK (194) listed fewer than 100 components reported in tobacco smoke and many of those listed were incorrect. Some of the early research on cigarette MSS composition, particularly the PAHs, was conducted at R. J. Reynolds Tobacco Company (RJRT)^b. Complete details of the experimental procedures and findings are available on the Internet at www.rjrtdocs.com.

The initial RJRT PAH investigation involved 11 PAHs in the MSS from non-filtered cigarettes (308, 312) [(see Table 1 in (323)]. Naphthalene, anthracene, pyrene, fluoranthene, and B[a]P, isolated in crystalline form, were characterized by UV absorption spectral data as well as by classical chemical means (mixture melting point, IR spectra, derivatization, and derivative properties). The other six PAHs were identified on the basis of agreement of their UV absorption spectra with those of authentic samples or with published UV data.

The second RJRT investigation involved the MSS from filter-tipped cigarettes (315, 329) [see Table 2 in (323)^c]. In that study 43 PAHs, including the 11 PAHs found in the initial study were identified (308, 312). Of the 43 PAHs, 14 were isolated in crystalline form and characterized by both UV spectral and classical chemical means [see Table 1 in (323)]. B[a]P, B[a]A, DB[a,h]A, and several other PAHs were also isolated in crystalline form from the CSC (308,312,329). The other 29 were identified from the agreement of their UV absorption spectra with those of authentic samples or with published spectra. B[a]P, B[a]A, and DB[a,h]A had been reported to be tumorigenic to mouse skin although the bioassay data for B[a]A were contradictory (88, 144).

Although much of the early research at RJRT R&D on the identification of PAHs in MSS and the effect of various tobacco blends and/or treatments on their MSS yields was summarized in several recent publications (323,341), other members of the US Tobacco Industry were also much

involved in similar research in the 1960s and 1970s. The following paragraphs provide a few examples of their early efforts:

At Philip Morris in 1963, ROBB *et al.* (301a) described the identification of 14 PAHs (naphthalene, fluorene, anthracene, 9-methylanthracene, phenanthrene, fluoranthene, pyrene, 1-methylpyrene, B[a]P, B[e]P), DB[a,h]A, benz[*e*]acephenanthrylene, perylene, benzo[*ghi*]perylene), biphenyl, and the aza-arene, carbazole, in cigarette MSS. Almost all the details in this 1963 Philip Morris in-house report were subsequently presented at the 1964 meeting of the Cooperation Center for Scientific Research Relative to Tobacco (CORESTA) meeting and published in 1965 (302). Also at Philip Morris, CARPENTER (49a) in 1964 described the per cigarette B[a]P yields from several commercial cigarettes; OAKLEY (265a) in 1965 reported the per cigarette B[a]P yields from cigarettes fabricated from different tobacco types (flue-cured, burley, Oriental); SEGURA (395a) in 1966 reported the contribution of cigarette paper to the per cigarette B[a]P yield; JOHNSON (180a) in 1965 described the effect of a tobacco additive, aluminum chloride, on the MSS B[a]P yield; and OAKLEY (265b) in 1966 determined the difference in per cigarette B[a]P yield in MSS and SSS.

At British American Tobacco Company (BAT) in 1966, CHAKRABORTY and THORNTON (51a) studied the effect of various additives on MSS PAHs. The changes in the per cigarette yields of a variety of PAHs were determined. They included: anthracene, B[a]A, benzo[*ghi*]fluoranthene, benzo[*k*]fluoranthene, B[a]P, B[e]P, chrysene, fluoranthene, fluorene, methylfluorene, phenanthrene, several alkylphenanthrenes, dimethylphenanthrene, pyrene, and several benzofluorenes.^d

Although studies on PAHs in MSS were conducted at RJRT and L&M in the 1960s, publications only dealt with analytical techniques. For example, in 1963 MOLD *et al.* (239a) at Liggett and Myers Tobacco Company (L&M) described the use of a compound, tetramethyluric acid, that complexes with polycyclic compounds. It was a procedure reminiscent of the finding of the water-soluble purine-PAH complex defined by WEIL-MALHERBE (470a), a finding subsequently developed into an alternative analytical method for the determination of PAHs and aza-arenes in tobacco smoke and other media by ROTHWELL and WHITEHEART (351–354). Although the study was not described as relating to tobacco smoke, CUNDIFF and MARKUNAS (72a) at RJRT in 1963 reported a titrimetric analysis of the nitro groups in numerous PAH:2,4,7-trinitrofluorenone complexes as a means to define the molecular weight of the PAH. All but one of the PAH:2,4,7-trinitrofluorenone complexes could be obtained from the PAH fraction of cigarette MSS. Of course, there were also methods developed for the in-house determination of specific PAHs, particularly B[a]P by BELL (20a) at Lorillard, OAKLEY and STAHR (266a) at Philip Morris, and WALKER (467) and STAMEY *et al.* (423, 424) at RJRT.

These and many other in-house reports on PAHs demonstrate that the early PAH research was not limited to

^bNumerous formal in-house reports and memoranda authored by RJRT R&D personnel are cited herein. Many have been published totally or in part in peer-reviewed journals and/or presented totally or in part at scientific conferences (Tobacco Chemists' Research Conferences, American Chemical Society Symposia on Tobacco and Smoke, CORESTA Conferences, etc.). Whether published, presented, or neither, copies of all RJRT reports cited are stored in various repositories such as the one in Minnesota. Their contents are available on the Internet address indicated. Experimental procedures used, data collected, and interpretations summarized here are described in detail in the reports cited.

^cDuring the editing of the page proof for Reference 323, the author (A.R.) failed to notice the omission of an item from Table 2. Unfortunately, Item 38, chrysene was omitted. The line should read:

No.	Polycyclic aromatic hydrocarbon	AC	PM	RJRT
38	Chrysene	–	D	x

^dAt the Internet address, <http://legacy.library.ucsf.edu/cgi>, by inserting the topic 'aromatic polycyclic hydrocarbons', one may access over 20 BAT and Brown and Williamson (B&W) memoranda by CHAKRABORTY, THORNTON, and others on PAHs in tobacco smoke.

academic or governmental laboratories or to laboratories at private institutions such as the Sloan-Kettering Institute, American Health Foundation, or Roswell Park Memorial Institute. Many of the above Tobacco Industry reports on PAHs may now be accessed at the Internet addresses cited in the references.

Additional PAHs – both tumorigenic and non-tumorigenic – were subsequently identified in CSC but the level of B[a]P in CSC could account for very little (90, 343, 344, 519) or less than 2% of the observed skin-painting effect (495, 519), the contribution of all the known tumorigenic PAHs in CSC could account for not much more than 3% of the observed effect. These findings led to the proposal by WYNDER and WRIGHT (519) that CSC contained a PAH that either possessed the same specific tumorigenicity as B[a]P but was present at about 50 times the B[a]P level or present in MSS was an unknown PAH that was “supercarcinogenic” compared to B[a]P, i.e., its specific tumorigenicity to mouse skin was 40 to 50 times that of B[a]P. After an 18-month search, WRIGHT, a colleague of WYNDER from the early to the late 1950s, concluded that neither type PAH was present in CSC. Subsequently, the absence of a “supercarcinogen” in CSC was confirmed by the identification of hundreds of PAHs in the PAH fraction of CSC by SNOOK *et al.* (419–422). Detailed examination of their lists does not reveal the presence of a PAH structurally different from any of those previously classified with regard to their specific tumorigenicity on mouse-skin painting.

No other CSC fraction possessed specific tumorigenicity to mouse-skin comparable to the PAH fraction. In the mid-1950s, the tumorigenicity of the *N*-nitrosamines in CSC was not an issue for several reasons: 1) The tumorigenicity of an *N*-nitrosamine was first defined in 1956 (233a), 2) The presence of *N*-nitrosamines in MSS was not suggested until the early 1960s (35a, 90a), and 3) Of the more than 300 *N*-nitrosamines tested for tumorigenicity, only one type not found in tobacco smoke – the *N*-nitrosoalkylureas – was found to be tumorigenic to mouse skin [e.g., see Appendixes A–D in (282b)].

Consideration of all the tumorigenic PAHs and their levels in CSC could account for no more than 3% of the observed biological activity in mouse skin-painting studies. In 1961, WYNDER and HOFFMANN (495) stated:

The polynuclear aromatic hydrocarbons are mainly formed during the combustion of tobacco. The tobacco of our standard cigarettes contains only very minute quantities of benzo(a)pyrene [*sic*] (0.02 ppm). A bioassay indicates that these polycyclic hydrocarbons of the condensate by themselves, however, can account for not more than 3 per cent of the total biological activity.

And in 1967, they reiterated their 1961 comment (513):

Without belaboring the point as to whether BaP as such contributes to the carcinogenicity of tobacco smoke condensate, we can certainly agree that the concentration of BaP may be regarded as an ‘indicator’ of carcinogenic PAH in tobacco smoke condensate . . . While BaP and other carcinogenic PAH can by themselves account for only a small portion of the total tumorigenic activity of cigarette smoke condensate, probably less than 2%, they are, nevertheless, of obligatory importance as tumor initiators.

HOFFMANN and WYNDER (166) reported that the major carcinogenicity of CSC resided in the CSC fraction containing the bulk of the PAHs. However, the levels in CSC of the non-alkylated carcinogenic PAHs could explain no

more than 1–3% of the observed activity. They also reported that the artificial doubling and tripling of the levels of the 17 known tumorigenic PAHs in CSC significantly increased the tumorigenicity of the CSC. However, their biological findings were contradicted by those of ROE (343, 344) and LAZAR *et al.* (214) who reported that increasing the level of B[a]P in CSC by a factor of 10 or 30, respectively, produced no increase in the specific carcinogenicity of the CSC. ROE (343, 344) also noted that the CSC level of B[a]P, despite its known tumorigenic potency, accounted for very little of the observed specific tumorigenicity of CSC to mouse skin. The opposite of these observations were the findings that potently tumorigenic PAHs such as DB[a,h]A on subcutaneous injection [DOBROVOLSKAIA-ZAVADSKAIA (88a)] and B[a]P on mouse skin painting [POEL *et al.* (282a)] exhibited a threshold value. WYNDER *et al.* (486) reported that mice skin painted with the equivalent of the B[a]P content of the CSC from over 500 current cigarettes developed no carcinomas. Rabbits were found to be even more resistant to higher dose levels of B[a]P.

Paralleling the research on the presence or absence of PAHs in cigarette MSS, their precursors in tobacco, their mechanism of formation, their contribution to laboratory animal tumorigenesis, and their possible involvement in the smoking-health issue was extensive research on ways to generate a “less hazardous” cigarette by removal of PAHs from or reduction of their per cigarette yields in MSS. To successfully resolve these questions, much pioneering research and development were initiated in late 1954 (323). When the question of the presence of PAHs in MSS was resolved, with many PAHs identified, and their per cigarette MSS yields determined, much effort was expended to develop technologies to reduce their MSS yield, particularly the yields of those PAHs reported to be tumorigenic to CSC-painted mouse skin. In the early 1960s, a “less hazardous” cigarette was defined on the basis of three criteria [see p. iii in (116); p. 372 in (500); pp. 503, 531 in (508)]: 1) the per cigarette yield of a specific toxicant has been lowered, 2) the ratio of the specific toxicant to MSS ‘tar’ has been lowered, and 3) the specific tumorigenicity of the MSS ‘tar’ as measured in the mouse skin-painting bioassay has been lowered. With the advent of meaningful tests for mutagenicity and genotoxicity, criterion 3 has been modified to include them.

The Tobacco Industry and non-Industry scientists investigated many additional approaches in the attempt to design a “less hazardous” cigarette [see Table 5 in (323), Table 14 in (336)]. Two examples of technologies that appeared to be promising but presented other toxicant problems were 1) the organic solvent-extraction of tobacco and 2) the use of oxidative additives.

The extraction concept was patterned after the findings of ROFFO (350) with one addition, the hexane extract of the tobacco was partitioned between hexane and aqueous ethanol to separate the flavorful compounds from those considered to be the PAH precursors, i.e., the phytosterols, the aliphatic hydrocarbons, the long-chained terpenoids (9, 10). When the extracted tobacco was smoked in cigarette form, its CSC showed much lower PAH levels than the control tobacco CSC (309, 314, 521) and reduced tumorigenicity (521). The flavorful components, when returned to the extracted tobacco and smoked in cigarette form,

contributed little to the total PAHs or B[a]P in the MSS [see Figure 1, Table 3, and accompanying text in (323)]. The solvent extraction removed from the tobacco not only many of the PAH precursors but also much of several potent anticarcinogens to such tumorigens as B[a]P and DB[a,h]A, e.g., long-chained aliphatic hydrocarbons, *d*-limonene, α -tocopherol, α - and β -1,5,9-trimethyl-12-(1-methylethyl)-4,8,13-cyclodecatriene-1,3-diol [(see Table 11 in (336)]. Thus, because of their removal from the tobacco, the anticarcinogens obviously could not be transferred to MSS during smoking. Before some of the problems were discovered, the investigation of the benefits supposedly derived from the organic solvent-extraction of tobacco led to several patents on the technology (10, 251, 253). The earliest major non-Tobacco Industry proponents of the contribution of the extraction technology to a “less hazardous” cigarette eventually dismissed it with the comment that the technology was “impractical both technically and economically” (494) and “of academic interest only” (489). Most of the findings on tobacco components that were, and tobacco components that were not, significant precursors of MSS PAHs in this early study were confirmed some years later by SEVERSON *et al.* (398). The problems arising from the organic solvent extraction included the increased levels of nitrate and the biopolymers cellulose, starch, and pectin in the solvent-extracted tobacco. These consequences increased the yields of nitric oxide, *N*-nitrosamines, and phenols (331a) in the MSS.

While nitrate addition reduced the per cigarette yields of FTC ‘tar’, MSS PAHs, phenols, and CSC tumorigenicity to mouse skin (164), it was subsequently shown, as predicted (165), to significantly increase the yields of MSS *N*-nitrosamines and nitrogen oxides (39). Thus, the recommendation to add nitrate to tobacco to reduce MSS PAHs was eventually replaced by the recommendation to use low-nitrate tobacco in the cigarette blend and/or remove nitrate from the tobacco (165). This reversal of recommendations was paralleled by another concerning the level of long-chained hydrocarbons such as *n*-hentriacontane in tobacco: Originally, it was proposed to reduce MSS PAHs by selection of tobaccos with low levels of such components or remove the PAH precursors by organic solvent extraction. This was replaced by a proposal to select tobaccos with high levels of such components (39).

By the early 1960s, several cigarette design technologies developed by the Tobacco Industry and used in commercial products were categorized as significant in their contribution to the “less hazardous” cigarette (493). Ultimately, the initial four design technologies (tobacco blend, effective and efficient filtration, reconstituted tobacco sheet (RTS), air dilution via cigarette paper porosity) were increased to eight [tobacco blend, filter tip, filter tip additives, RTS, paper additives, expanded tobacco, air dilution (paper porosity), air dilution (filter tip perforation)]. Their significance was recognized in “less hazardous” cigarette design by the NATIONAL CANCER INSTITUTE (NCI) (245)^e and the

^eAll eight cigarette design technologies eventually classified as significant by NCI, several US Surgeon Generals, and other investigators on the basis of the 10-year NCI Smoking and Health Program on the “less hazardous” cigarette had been incorporated into one or more US commercial cigarette products prior to the first meeting of the Tobacco Working Group formed in 1968 for the NCI program. In other words,

US Surgeon General [see Table 6 in (323), Table 15 in (336)] (445–453). It should be noted that the first two technologies considered significant were used before 1954. Tobacco or tobacco blend selection had been used since 1913, even before the first tumors were induced in a laboratory animal by skin painting with a solution of coal tar (522). RTS was introduced into cigarette blends in 1953 when little was known about the chemical composition or biological properties of tobacco smoke (194) or the effect of RTS inclusion in the blend on them. When knowledge of tumor induction with CSC and the presence of PAHs including B[a]P became available, it was shown that use of these two technologies resulted in a cigarette whose MSS was in compliance with that in the definition of a “less hazardous” cigarette (336).

Of course, the initial thrust of this across-the-board reduction was aimed at reducing the MSS ‘tar’ delivery because of extrapolation by WYNDER *et al.* (516) of their 1957 mouse-skin bioassay findings:

Although it is difficult to estimate a comparable exposure level for man, the human data in line with the animal data indicate that a reduction in total tar exposure will be followed by a decrease in tumor formation. For this reason, measures directed toward this reduction are of utmost importance . . . The minimum dose of tar capable of producing papillomas in mice is about one third, of producing cancer one half, that of the optimum dose . . . The practical implications of these data and their relationship to the human cancer problem have been emphasized.

In his 1957 testimony during the filter-tipped cigarette hearings, WYNDER reiterated this opinion that reducing ‘tar’ exposure dose by 40% to 50% would substantially reduce lung cancer induction in smokers (483):

Examination of the sales-weighted average ‘tar’ delivery for US commercial cigarettes reveals that the 40% to 50% reduction in MSS ‘tar’ delivery considered vital by WYNDER in 1957 was achieved in the late 1960s, i.e., a reduction from 38–39 mg/cig to 19–20 mg/cig. Further examination reveals that by the early 1980s, the sales-weighted average ‘tar’ was reduced to about 12 mg/cig, i.e., an additional 40% reduction had been achieved [see Figure 3 in (323)]. Corresponding reductions in the per cigarette yields of total PAHs in general, B[a]P in particular (470), and nicotine were also observed. These reductions were also accompanied by a reduction in the specific tumorigenicity (mouse-skin painting) of the MSS CSC (448).

By year-end 1963, 91 of the 97 PAHs identified in MSS were reported in the published literature. Six PAHs, identified in MSS by RODGMAN and COOK (329), had not been reported publicly at that time. However, by 1970, identification in MSS of all but one (cholanthrene) of the 97 had been reported. Despite the availability of such information, only 18 MSS PAHs were discussed by the Advisory Committee in its 1964 Report to the US Surgeon General, 13 as mainstream CSC components and five as carbon black components (445). The detailed discussion of so few MSS PAHs and citation of so few publications was done despite the fact the Committee had been provided with a detailed Philip Morris monograph on tobacco and smoke composition, a monograph that listed 61 PAHs

from 1968 to 1978, no new design technology was generated in the NCI Smoking and Health Program on the “less hazardous” cigarette.

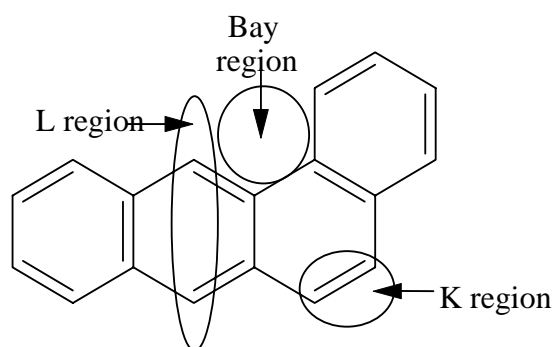


Figure 1. The L region, K region, and bay region of benz[a]anthracene

identified in tobacco smoke plus many pertinent published references to them (278, 323). The Advisory Committee did note, however, that 27 other non-tumorigenic PAHs – none specifically named – had been identified in tobacco smoke. The 27 unnamed PAHs had to include several of those PAHs, e.g., naphthalene, anthracene, phenanthrene, fluoranthene, pyrene, which had been reported to significantly inhibit the action of potently tumorigenic PAHs such as B[a]P and DB[a,h]A in laboratory animal studies. Of the 97 PAHs known to him, RODGMAN (323) discussed the 43 PAHs identified at RJRT plus 34 other PAHs reported in the literature in numerous reports between 1954 and 1964 and in a summary 1964 report on 10-year research on cigarette MSS (317). Interestingly, Chapter 6, in the Advisory Committee's report on cigarette smoke chemistry and the tumorigenic PAHs, was primarily authored by FIESER, one of the two eminent American PAH authorities at that time.

THE CATALOGUE OF POLYCYCLIC AROMATIC HYDROCARBONS: A REASON FOR IT

For over half a century, numerous theories have been advanced in attempts to explain the relationship between the tumorigenicity of polycyclic aromatic hydrocarbons (PAHs) in treated laboratory animals and a variety of their structural properties, including such properties as their K-, L-, and bay-regions, electron distribution, bond orders, bond strengths, resonance, octanol-water partitioning, and the like, Figure 1. Such studies were triggered by the discovery that certain PAHs when administered to laboratory animals via skin painting or subcutaneous injection induced carcinomas or sarcomas, respectively. DB[a,h]A, synthesized independently by CLAR (58) and FIESER and DIETZ (105a) in 1929, was shown to be a potent tumorigen to laboratory animals by KENNAWAY and HIEGER (186). Shortly thereafter, COOK *et al.* (64) isolated several PAHs from coal tar, characterized one of them as the previously unknown benzo[a]pyrene (B[a]P), and demonstrated that it too was a potent tumorigen to laboratory animals (18). Over the next two decades, the first demonstrations of the carcinogenicity of two pure compounds, DB[a,h]A and B[a]P, led to the synthesis and subsequent testing for tumorigenicity in laboratory animals of literally hundreds of PAHs and their alkyl derivatives plus other derivatives.

During this time, the variation in biological responses observed with laboratory animals to individual PAHs eventually led to numerous unacceptable extrapolations of the results to PAH-exposed humans. To put the laboratory animal-to-human extrapolation in perspective, SHEAR and LEITER (404) in 1941 issued a list of pertinent factors to be considered in such an extrapolation. Despite a diminution in PAH synthesis and tumorigenicity research during World War II, the wealth of experimental data available in the late 1940s – early 1950s on the high-to-slight tumorigenic potency of some PAHs and the non-tumorigenicity of other PAHs induced investigators to seek reasons for the observed differences in tumorigenicity and to attempt to develop explanations for them. Among those involved in the generation of the major early theories on the relationship between PAH structural properties and PAH tumorigenicity or lack of it were COULSON (71); PULLMAN and PULLMAN (283); DAUDEL and DAUDEL (77); FIESER *et al.* (102) and FIESER (103); and LACASSAGNE *et al.* (204). Much meaningful input to these theories was provided by other investigators such as PAULING (275a) in the USA, BOYLAND, WEIGERT, and MOTTRAM (35b) in the UK, and BUU-HOÏ in France [see more than 30 BUU-HOÏ references listed in (204)]. More recent studies include those by HERNDON *et al.* (150, 231), RUBIN (356), TROSKO (440), L. ZHANG *et al.* (529), and Y. ZHANG, a graduate student under HERNDON (530).

Because it was issued at the beginning of the extensive research on the composition of tobacco smoke with particular emphasis on the nature and levels of the PAHs in it, it is interesting to examine the lengthy 1955 review by PULLMAN and PULLMAN (283) on the relationship between electronic structure and the tumorigenicity of a number of benzenoid hydrocarbons. Their publication was a detailed update of the 1953 review by COULSON (71) and included much data generated in the interim. The PULLMANS used calculations based on three theoretical indexes of the K and L regions of the aromatic hydrocarbons. The indexes included Carbon Localization Energy (CLE), Bond Localization Energy (BLE), and *Para* Localization Energy (PLE) [see Table 1 in (283)]. The PULLMANS, by use of their CLE, BLE, and PLE calculations pertinent to the K and L regions in the PAHs, also attempted to relate the structures of various PAHs and their alkylated derivatives not only to their tumorigenicity but also to their rate of reaction in certain well-known reactions, e.g., Diels-Alder reaction with maleic anhydride, reaction with osmium tetroxide, reaction with lead tetraacetate, photo-oxidation. Table 2 lists the hydrocarbons discussed by the PULLMANS in 1955 with an indication of those, 34 in all, which were identified in tobacco smoke before and after 1955.

The PULLMANS did introduce into their discussion various PAH metabolites, their diols and phenols, but not the epoxides which were unknown at that time. Even though it had been known since 1951 (426), no explanation was offered for the inhibition of the activity of a potently tumorigenic PAH by co-administration of a weakly tumorigenic or non-tumorigenic PAH. Lastly, of course, neither the PULLMANS nor COULSON discussed the fact that a bioassay finding with a highly susceptible strain or species of laboratory animal administered an individual PAH in an excessive dose has little relationship to the

Table 2. Benzenoid hydrocarbons discussed by PULLMAN and PULLMAN (283)

Aromatic hydrocarbon discussed	CAS RN	No. in PAH list in Table 6	No. in Pullman and Pullman	Considered tumorigenic ^a in 1955
<i>Monocyclic</i>				
Benzene ^b	71-43-2	—	I	no
<i>Bicyclic</i>				
Naphthalene	91-20-3	1	II	no
<i>Tricyclic</i>				
Anthracene	120-12-7	157	III	no
Phenanthrene	85-01-8	173	IV	no
<i>Tetracyclic</i>				
Naphthacene	92-24-0	264	VII	no
Benz[<i>a</i>]anthracene	56-55-3	266	VI	?
Benz[<i>a</i>]anthracene, 2,10-dimethyl-	—	—	XLIII	?
Benz[<i>a</i>]anthracene, 7,12-dimethyl-	57-97-6	270	XLII	yes
Benz[<i>a</i>]anthracene, 7-methyl-	2541-69-7	—	XLIV	yes
Benzo[<i>c</i>]phenanthrene	195-19-7	290	V	yes
Benzo[<i>c</i>]phenanthrene, 1,2-dimethyl-	—	—	XLVIII	no
Chrysene	218-01-9	292	VIII	?
Chrysene, 2,3-dimethyl-	—	294 ^c	XLIX	no
Triphenylene	217-59-4	307	X	no
Pyrene	129-00-0	311	IX	no
<i>Pentacyclic</i>				
Benzo[<i>b</i>]chrysene	214-17-5	414	XXIII	no
Benzo[<i>c</i>]chrysene	194-69-4	—	XIII	yes
Benzo[<i>g</i>]chrysene	196-78-1	—	XIV	yes
Pentacene	135-48-8	415	XVIII	no
Benzo[<i>a</i>]naphthacene	226-88-0	416	XVII	no
Dibenz[<i>a,h</i>]anthracene	53-70-3	418	XII	yes
Dibenz[<i>a,j</i>]anthracene	224-41-9	419	XV	yes
Pentaphene	222-93-5	420	XIX	no
Perylene	198-55-0	421	XXV	no
Picene	213-46-7	427	XXI	no
Benzo[<i>b</i>]triphenylene	215-58-7	428	XX	no
Benzo[<i>a</i>]pyrene	50-32-8	430	XI	yes
Benzo[<i>a</i>]pyrene, 2-methyl-	—	437–438 ^d	XLVII	yes
Benzo[<i>a</i>]pyrene, 3-methyl-	—	—	XLVII	yes
Benzo[<i>a</i>]pyrene, 5-methyl-	—	—	XLVII	yes
Benzo[<i>a</i>]pyrene, 6-methyl-	2381-39-7	—	XLVII	yes
Benzo[<i>a</i>]pyrene, 7-methyl-	63041-77-0	—	XLVII	yes
Benzo[<i>a</i>]pyrene, 8-methyl-	63041-76-9	—	XLVII	no
Benzo[<i>a</i>]pyrene, 9-methyl-	—	—	XLVII	no
Benzo[<i>e</i>]pyrene	192-97-2	440	XVI	no
Dibenzo[<i>b,g</i>]phenanthrene	195-06-2	—	XXIV	no
Dibenzo[<i>c,g</i>]phenanthrene	188-52-3	—	XXII	no
Benzo[<i>j</i>]aceanthrylene, 1,2-dihydro-3-methyl- ^e	56-49-5	449	XLV	yes
<i>Hexacyclic</i>				
Anthra[1,2- <i>a</i>]anthracene	195-00-6	—	XXXV	no
Benzo[<i>c</i>]pentaphene	222-54-8	—	XXXVII	no
Benzo[<i>rsf</i>]pentaphene	189-55-9	482	LIV	(yes) ^f
Benzo[<i>pqr</i>]picene	189-96-8	—	LVII	no
Dibenzo[<i>b,def</i>]chrysene	189-64-0	493	XXVII	yes
Dibenzo[<i>b,k</i>]chrysene	217-54-9	—	XXXVI	no
Dibenzo[<i>c,mno</i>]chrysene	196-28-1	—	LVI	no
Dibenzo[<i>def,mno</i>]chrysene	191-26-4	494	XXXI	no
Dibenzo[<i>def,p</i>]chrysene	191-30-0	501	XXVI	yes
Dibenzo[<i>a,j</i>]naphthacene	227-04-3	504	XXXIII	no
Dibenzo[<i>a,l</i>]naphthacene	226-86-8	—	XXXIV	no
Dibenzo[<i>fg,op</i>]naphthacene	192-51-8	506	XXIX	no
Naphtho[1,2,3,4- <i>def</i>]chrysene	192-65-4	508	XXXVIII	?
Naphtho[2,1,8- <i>qra</i>]naphthacene	196-42-9	510	XXX	no
Naphtho[1,2- <i>b</i>]triphenylene	215-26-9	511	XXXII	no

Table 2 (cont.)

Aromatic hydrocarbon discussed	CAS RN	No. in PAH list in Table 6	No. in Pullman and Pullman	Considered tumorigenic ^a in 1955
<i>Heptacyclic</i>				
Benzo[<i>a</i>]naphtho[8,1,2- <i>lmn</i>]naphthacene	190-01-2	—	LV	no
Dibenzo[<i>fg,qr</i>]pentacene	197-74-0	—	XL	no
<i>Octacyclic</i>				
Dinaphtho[1,2- <i>b:1,2-k</i>]chrysene	214-13-1	—	XXXIX	no
Naphthaceno[2,1,12,11- <i>opqra</i>]naphthacene	188-42-1	—	LVIII	? ^g
Phenanthro[1,10,9,8- <i>opqra</i>]perylene	190-39-6	—	XLI	no
<i>Nonacyclic</i>				
Dinaphtho[1,2- <i>b:1,2-n</i>]perylene	—	—	XXXVIII	no
<i>Decacyclic</i>				
Pentacenopentacene	—	—	LIX	? ^g

^a Tumorigenic in mouse skin-painting study.

^b Benzene was reported as a component of the vapor phase of tobacco smoke in 1955 by RESNIK and HOLMES (298a) and LAURENE (212a).

^c A dimethylchrysene was reported in tobacco smoke, but the positions of the methyl groups were not defined.

^d At least two methylB[*a*]Ps were reported in tobacco smoke, but the position of the methyl group in each case was not defined.

^e This PAH is not totally benzenoid; its structure includes a cyclopentanoid ring.

^f In 1955, the tumorigenicity of dibenzo[*rsf*]chrysene had not been determined; later it was reported to be tumorigenic.

^g Although no calculation was made on this PAH, PULLMAN and PULLMAN (283) predicted it would be tumorigenic.

Table 3. Polycyclic hydrocarbons reported in tobacco smoke by year-end 1955

Hydrocarbon	References issued in the year			
	1947	1953	1954	1955
Acenaphthylene ^a		67	68, 70	69, 221
Azulene ^{a,b}	173			221
Anthracene		67	61, 68	69, 219, 221, 395
Anthracene, 2-methyl-				69
Benz[<i>a</i>]anthracene				219, 227
Benzo[<i>ghi</i>]perylene			68	69, 221, 227
Benzo[<i>a</i>]pyrene			61, 68, 70, 217	6, 48, 100, 184, 221, 395, 518
Benzo[<i>e</i>]pyrene				219
Dibenzo[<i>def,mno</i>]chrysene			68	69, 221
Fluoranthene ^a			68	69, 221
Naphthalene				395
Naphthalene, 2-methyl-				69
Phenanthrene			68	69, 221
Pyrene		67	61, 68	69, 219, 221, 227

^a Molecule has a cyclopentanoid ring, thus it was not considered by PULLMAN and PULLMAN (283).

^b Molecule does not possess a benzenoid structure.

situation where a human is exposed by a different administration route to a mixture of PAHs with various degrees of tumorigenicity plus other known anti-tumorigenic compounds.

By year-end 1955, very few of the PAHs considered by the PULLMANS had been reported as tobacco smoke components. More had been identified in other sources such as air pollution. In the following discussion, the comments in the early 1950s about the inadequacy of the evidence indicating the presence of B[*a*]P in tobacco smoke (104) are disregarded. Table 3 lists the PAHs reported in tobacco smoke at that time. Of the 14 PAHs reported, only eight were included by the PULLMANS in their assessment: naphthalene, anthracene,

phenanthrene, B[*a*]A, B[*a*]P, B[*e*]P, dibenzo[*def,mno*]chrysene, naphthalene, phenanthrene, and pyrene. Of course, only one of the eight, B[*a*]P, was considered at that time a significant and potent tumorigen to mouse skin. At that time, the tumorigenicity of B[*a*]A was questioned, and still was questioned in the mid-1980s (88).

As noted previously, PULLMAN and PULLMAN not only updated the electronic structure-tumorigenicity information generated after the COULSON 1953 review but also attempted to extend the theory to alkyl-PAHs. Examination of their review reveals that they discussed, in addition to 1,2-dihydro-3-methylbenz[*j*]aceanthrylene, a total of twelve alkyl-PAHs (see Table 3). It is obvious from their discussion that the prediction of tumorigenicity for most of these 12 PAHs was not calculated but derived from published biological data. However, examination of the biological data in HARTWELL (144) and SHUBIK and HARTWELL (408) indicates that at least 64 totally benzenoid alkyl-PAHs had been tested for tumorigenicity by 1955. Several 1,2-dihydromethylbenz[*j*]aceanthrylenes had been tested for tumorigenicity by 1955, but they were not included in our count of 64. This raises the question: Why was the prediction not calculated for more of the 64 alkyl-PAHs, the tumorigenicity of which was known at that time (144, 408)? PULLMAN and PULLMAN noted:

It must be acknowledged that the extension of the theory to substituted derivatives of polycyclic hydrocarbons is at present far from having achieved a completely consistent and satisfactory form.

Many of the more recent theories on the relationship between PAH structural properties and tumorigenicity suffer somewhat from this and other deficiencies [cf. HERNDON *et al.* (150, 231), RUBIN (356), TROSKO (440), L. ZHANG *et al.* (529), and Y. ZHANG (530)]. Much studied in recent years has been the application of the quantitative structure-activity relationship (QSAR) method to PAHs.

While many theories have involved the relationships between observed laboratory-derived biological data on individually administered PAHs and their structural

elements, do they speak to the exposure situation experienced by humans? Whether the exposure is by inhalation of air pollutants or tobacco smoke, by ingestion of foodstuffs or beverages, by dermal contact, or by a combination of the exposures, very few of any human exposures involve exposure to a single PAH similar to the exposure of laboratory animals treated with a single PAH by skin painting or subcutaneous injection. One such example of human exposure to a single PAH was the past use of naphthalene as the major ingredient in mothballs.

Numerous PAHs have been either completely or partially characterized in many air pollutants, foodstuffs, beverages, and contact tars and dusts. Of all the products to which humans are exposed, none has been characterized to the extent of tobacco smoke. Nearly 4800 components have been identified in it, nearly twice as many as in the next consumer product, coffee, subjected to detailed compositional analysis. Of the identified tobacco smoke components, about 11% were either completely or partially identified as PAHs. It should also be noted that in the detailed examination of tobacco smoke, the 4800 identified components account for over 98% of the weight of cigarette MSS. It has been estimated, based on detailed gas chromatograms, that the number of actual components in cigarette MSS may be 12 to 20 times the number of identified ones (465).

Of the more than 500 PAHs either completely or partially identified in cigarette MSS, relatively few PAHs, originally 13 in all, were repeatedly defined as significant tumorigens (152, 167, 174). Eventually, the International Agency for Research on Cancer (IARC) redefined the tumorigenicity of chrysene. Thus, it was deleted from all subsequent lists (153, 154, 156, 157, 268) except one (106). MSS is not the only source of most of the 12 PAHs still considered as significant tumorigens in cigarette MSS. Except for 5-methylchrysene, most have also been identified as significant PAH components of gasoline and diesel engine exhaust gases (132, 496) and many common foodstuffs and beverages (122, 232).

When one is dealing with a complex mixture, which in turn contains an assortment of PAHs ranging from bicyclic to decacyclic, one cannot extrapolate the biological effect observed by administration of an individual PAH to the biological effect of that PAH in such a complex mixture. It has long been known from laboratory studies that certain non-tumorigenic or slightly tumorigenic PAHs when administered by skin painting or subcutaneous injection in an equimolar dose level with a highly tumorigenic PAH partially or totally inhibit its tumorigenicity. Few studies have been done to determine the effect of a non- or low-tumorigenic PAH on the tumorigenicity of a highly tumorigenic PAH when its level greatly exceeds that of the potent tumorigen. Also, there are differences in the classification of the potency of the tumorigenicity of some PAHs. For example, B[a]A is classified by some (174) as a potent or significant tumorigen but by others as only slightly tumorigenic (88)^f.

^f One of us (A.R.) was involved in the late 1940s in a comparison of the tumorigenicities of several PAHs (B[a]P; DB[a,h]A; B[a]A) administered by skin painting or by subcutaneous injection. Equimolar doses of each PAH were administered to groups of mice (50 per group) so that the % Tumor Bearing Animals (TBA) with B[a]P and DB[a,h]A were approximately 80%. The equimolar dose of B[a]A, a commercial sample, m.p. 166–167 °C, gave only 2% TBA, i.e., one mouse with tumor.

The list of either totally or partially identified PAHs in CSC gradually increased but in the mid-1970s the massive definitive PAH study by United States Department of Agriculture (USDA) personnel in Athens, GA increased the number of known PAHs in CSC to well over 500 (416, 417–422). Although not isolated individually, their identifications, whether total or partial, have generally been accepted across the board.

Numerous authors, including HOFFMANN and HECHT (152), listed the PAH dibenzo[a,l]pyrene as a significant tumorigen in tobacco smoke. However, HECHT eventually stated (145) that “the presence in cigarette smoke of dibenzo[a,l]pyrene, a highly carcinogenic PAH, had not been confirmed”. One should weigh the comment by HECHT against the current status of defined MSS composition. Since the appreciable decline in detailed tobacco smoke composition studies after the late 1970s, no individual investigator or no research group has reported the confirmation of the identities of many of the PAHs (419–422), aza-arenes (418, cf. 362), nitrogen-containing components (147), or ether- (264) and water-soluble components (391) reported in cigarette MSS in the 1970s. While many components have been confirmed by other investigators at the same institution as the authors, examination of the post-1980 literature indicates that the identities of nearly half the new components described in the above-mentioned studies have not been confirmed by investigators at other institutions. Because of such a situation, would HECHT also discount their presence in cigarette MSS in the same way as he discounted the presence of dibenzo[a,l]pyrene?

While most of the past theories have attempted to define the relationship between structural properties of the PAHs and their specific tumorigenicity as measured individually in skin-painting studies, little has been done to explain the behavior of a PAH when it is present in a complex mixture which includes a host of PAHs some of which are known anti-tumorigens as well as numerous known non-PAH anti-tumorigens (101).

It has been known for over 60 years that co-administration of a potently tumorigenic PAH with an equimolar quantity of a non-tumorigenic PAH often results in substantial reduction in % tumor bearing animals (%TBA).

In 1953, COULSON noted [see p. 51 in (71)]:

The action of inhibitors may be thought of as a competition between the carcinogenic and noncarcinogenic compounds for available sites on the enzyme. If sufficient noncarcinogenic molecules are able to occupy suitable sites, then the irreversible mutation cannot occur. We can see that inhibitors, in order to compete with the carcinogenic compounds, should themselves possess a K-region.

Some of the PAHs that substantially reduce or totally inhibit the tumorigenicity of several of the most potent tumorigens known are listed in Table 4. Obviously, neither naphthalene nor anthracene has a K-region, a requirement proposed by COULSON for the inhibitory property.

Purification of the B[a]A by complex formation and column chromatography on alumina not only increased the melting point and diminished the m.p. range (167.2–167.5 °C), but improved the UV absorption spectrum. An equimolar dose of the purified B[a]A gave 0% TBA; quintupling the dose gave 0% TBA. The following question remained unanswered: Was the 2% TBA with the commercial sample due to the B[a]A or to a contaminant?

Table 4. Inhibition of tumorigenicity of potentially tumorigenic PAHs by non-tumorigenic or weakly tumorigenic PAHs

PAH ^a	CAS No.	Effective against	References
Naphthalene	91-20-3	B[a]P, DB[a,h]A	72
Anthracene	120-12-7	B[a]P, DB[a,h]A	72
Phenanthrene	85-01-8	DMB[a]A	82, 410
Fluoranthene	206-44-0	B[a]P, DMB[a]A	82, 410, 411
Pyrene	129-00-0	DB[a,h]A, DMB[a]A	82, 410, 411
Benz[a]anthracene	56-55-3	B[a]P, DB[a,h]A	426, 509
Benzo[e]pyrene	192-97-2	B[a]P, DB[a,h]A, DMB[a]A	82, 410, 411
Benzo[b]triphenylene	215-58-7	MC ^b , DB[a,h]A, DMB[a]A	82, 409, 411

^a Each PAH listed is a component of cigarette MSS. ^b MC = 3-methylcholanthrene = 1,2-dihydro-3-methylbenz[*j*]aceanthrylene.

Table 5. Levels of PAH classes in cigarette mainstream smoke

PAH category	Assumed approximate mol. wt.	Mainstream smoke yield ^a		
		Yield, ng/cig ^b	Approximate nanomoles ^c	Nanomolar ratio, PAH:B[a]P
Bicyclic	128 ^d	4140 (77.1)	32.3	293
Tricyclic	178 ^e	720 (13.4)	4.0	36
Tetracyclic	228	420 (7.9)	1.8	16
Pentacyclic	278	72 (1.3)	0.26	2.4
B[a]P	252	27 (0.49) ^f	0.11	1.0
Non-B[a]P pentacyclic	278	45 (0.81) ^f	0.16	1.5
Hexacyclic	328	14 (0.3)	0.04	0.36
TOTALS		5366 (100.0)		

^a Data reported by HOFFMANN and WYNDER (163) from a nonfiltered cigarette, total particulate matter = 36.8 mg/cig, were averaged with data reported by RODGMAN and COOK (329) for a filtered commercial cigarette, total particulate matter = 37.5 mg/cig.

^b Values in parentheses represent the fraction % of the PAH category in the total PAH fraction.

^c Nanomoles calculated with the approximate molecular weights in Column 2.

^d The molecular weight of naphthalene = 128, that of indene = 116. It is realized that the average molecular weight of the bicyclic PAH mixture will differ slightly from those of the parent PAH because of the presence of numerous homologs (methylnaphthalenes, dimethylnaphthalenes, etc.).

^e The presence of tricyclic PAH homologs results in molecular weight slightly different from 178.

^f The sum of the fraction % of B[a]P and the fraction % of non-B[a]P pentacyclic PAHs equals 1.3%.

While many of the inhibition studies were conducted with the tumorigenic and inhibiting PAHs administered in equimolar quantities, it should be remembered that this is not the case in the PAH mixture in CSC. Table 5 is derived from CSC PAH data presented by HOFFMANN and WYNDER (163,165) and RODGMAN (329). The per cigarette yield data in Table 5 were the averages of the data generated from two different commercial American cigarettes. One was unfiltered and yielded 36.8 mg/cig of total particulate matter (TPM) (163); the other was a filtered cigarette that yielded 37.5 mg/cig of TPM (329). The disparity between the relative yields in each category was less than 5%.

In the early structure-biological activity studies, PAHs with a pentacyclic ring were not included in the discussion of most theories but pentacyclic compounds in which the pentacycle contained nitrogen were, i.e., benzacridines (71, 204). In the discussion of his theory, COULSON (71) did mention several cyclopentanoid compounds: Six benzacridines and two PAHs, 2,3-dihydro-1*H*-benzo[*a*]cyclopent[*h*]anthracene and 10,11-dihydro-9*H*-benzo[*a*]cyclopent[*i*]anthracene.

In her 1996 thesis, ZHANG (530) noted the numerous sources of PAHs to which humans are exposed, e.g., air pollutants, foodstuffs and beverages, effluents from factories, vehicles, and heat and power sources. ZHANG particularly stressed tobacco smoke, its complexity, and some of the PAHs contained therein:

Tobacco smoke is a complex mixture which is estimated to contain at least 150 compounds in the gas phase and more than 2000 compounds have been identified in the particulate phase. Table 1^a lists some PAHs that exist in the particulate phase of cigarette smoke.

^a In her Table 1, ZHANG (530) listed 19 MSS PAHs reported in 1978 by HOFFMANN *et al.* (160a).

Unfortunately, the inconsistent use of PAH nomenclature sometimes makes it difficult to follow the phases of the study by ZHANG [cf. Table 7 and Appendix A in (530)].

Another study, recently initiated by MARTIN *et al.* (234a), involved an attempt to develop a meaningful relationship between PAH structure, chemical properties, and biological properties, specifically the effect of PAHs on specific tumorigenicity in skin painting. Reported for naphthalene- and pyrene-related PAHs were the following molecular parameters: The measured and calculated log of the octanol-water partition coefficient (MlogP, ClogP), molecular volume (MgVol), calculated molar refractivity (CMR), and the number of valence electrons (NVE). The second phase of the study involves similar data for anthracenes, phenanthrenes, and indenenes (336a). All the PAHs in the first two phases of this study (234a,336a) are reported components of cigarette MSS. The ultimate goal is to use these data to facilitate a quantitative structure-activity relationship (QSAR) on MSS PAHs. If such a meaningful relationship can be derived for the more than 500 MSS PAHs, then it probably can be applied to any PAH from any source.

As a prelude to this attempt to develop a possibly reasonable explanation for the PAH structure-tumorigenicity relationship, the PAHs completely or partially identified in cigarette smoke have been catalogued. In Tables 6 and 7, the PAHs are categorized as bicyclic, tricyclic, tetracyclic, etc. with each group subdivided into all-benzenoid PAHs and cyclopentanoid-benzenoid PAHs. For each PAH, the nomenclature used in Tables 1, 4, and 5 is the most recent proposed by the International Union of Pure and Applied Chemistry (IUPAC).

The tobacco smoke PAH references cited in Table 6 are not necessarily all that are available, particularly for those PAHs such as B[a]P and DB[a,h]A, which have been the subject of much research and discussion for over half a century. In most cases, included is a reference to the publication or presentation by the investigator(s) who first reported a particular PAH in MSS. References of articles and/or presentations on specific PAHs that contained evidence later criticized are included plus references to the misinterpretations or errors. The criticism by FIESER (104) in 1957 of the shortcomings of the evidence (6, 46–48, 69) supposedly indicating the presence of B[a]P in cigarette smoke has already been mentioned. Two other notable situations involved 1,2-dihydrobenz[j]aceanthrylene (cholanthrene) and dibenzo[def,p]chrysene (formerly named dibenzo[a,l]pyrene, initially 1,2,3,4-dibenzopyrene). These two PAH identifications, based solely on UV spectral data, were found to be incorrect. In their study, RODGMAN and COOK (329) incorrectly defined a PAH as 1,2-dihydrobenz[j]aceanthrylene (cholanthrene). In the massive study by USDA personnel on the identification of MSS PAHs, 1,2-dihydrobenz[j]aceanthrylene was not among the several benzocyclopentantracenes reported (419, 422). The other incorrectly characterized PAH was dibenzo[def,p]chrysene. For its identification, not only RODGMAN and COOK (329) but also BONNET and NEUKOMM (33), LYONS and JOHNSON (230), LYONS (228), WYNDER and WRIGHT (519), and PYRIKI (286) relied on published UV spectral data purportedly those of synthetic dibenzo[def,p]chrysene (dibenzo[a,l]pyrene). However, in 1966, LAVIT-LAMY and BUU-HOI (213) determined that the published UV spectral data were not those of dibenzo[a,l]pyrene but of the isomeric dibenz[a,e]aceanthrylene (dibenzo[a,e]fluoranthene), generated during the supposed synthesis of dibenzo[a,l]pyrene. The authentic dibenzo[def,p]chrysene (dibenzo[a,l]pyrene) was identified in MSS in 1977 (419), but its MSS level was not reported.

Some authorities insist that the B[a]P and 4-(methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK) in cigarette smoke are the major causes of lung cancer in cigarette smokers (HECHT, 145; HECHT and HOFFMANN, 146a; HOFFMANN and HECHT, 152; WORLD HEALTH ORGANIZATION, 475a) despite the following: 1) Neither B[a]P nor any other PAH in CSC either individually or in combination with the other PAHs in CSC can explain more than a few percent of the biological response observed in skin painting with CSC (DRUCKREY, 90; ROE, 343, 344; WRIGHT and WYNDER, 478; WYNDER, 483; WYNDER and HOFFMANN, 490, 495, 514a, 514b, 519); 2) Neither B[a]P nor any other PAH in CSC either individually or in combination with the other PAHs and assorted promoters (phenols) in CSC can

explain more than a few percent of the biological response observed in skin painting with CSC (508); 3) In general, the *N*-nitrosamines in CSC are not tumorigenic to mouse skin but are organ-specific tumorigens (PREUSSMANN and STEWART, 282b)[§], a point stressed in numerous reviews issued between the mid-1960s and the late 1990s on *N*-nitrosamines (RODGMAN, 321a) and recognized by HOFFMANN and HECHT [see p. 75 in (152)]; 4) NNK has never been shown to induce lung cancer in a laboratory animal by inhalation (152).

While the minor contribution of B[a]P to the tumorigenicity of CSC to mouse skin has been recognized since the mid-1950s (518, 519), its presence in CSC has elicited continued interest since that time. Examination of the references to various smoke components reveals an interesting fact about B[a]P: When all the cigarette smoke components are tabulated with regard to similar selection of references across the board, very few tobacco smoke components exceed B[a]P in the number of pertinent references available. Obviously, the smoke component discussed most in publications and presentations between the mid-1950s and 2005 was nicotine. Next was acetaldehyde, followed by B[a]P.

Another interesting fact about B[a]P is that, despite its minimal contribution to mouse-skin tumorigenicity from CSC, almost every year since the mid-1950s there has been at least one publication on a new and/or improved method to quantitate the yield of B[a]P in MSS. In 2004, CORESTA published its recommended method for the determination of B[a]P in tobacco smoke (70a). Much emphasis has been placed on the determination of B[a]P in the MSS from fewer and fewer cigarettes. Before the advent of all the newly introduced and subsequently improved spectral and chromatographic systems, estimations of individual PAHs required the CSC from many cigarettes. For example, in their studies on the effect of various treatments of tobacco on the PAHs in MSS, RODGMAN and COOK (309, 314, 327, 330, 331) chemically analyzed the MSS from 3600 cigarettes for each control and treated sample. For the MSS PAH analyses in the 50 treated and control samples described in (314), more than 183,000 cigarettes were smoked, the condensate collected, and processed. Nowadays, only a few cigarettes are needed for similar analyses. To permit comparison of the chemical data with the biological findings of WYNDER *et al.* (488), the smoking procedure used by them was duplicated in the RODGMAN-COOK studies in the 1950s, i.e., the cigarettes on a manifold were machine smoked (35-mL puff volume, 2-sec puff duration, 3 puffs/min) with a collection system that duplicated the one described by WYNDER *et al.* (488). This smoking regime differed from the usual 35-mL puff volume, 2-sec puff duration, 1 puff/min described by BRADFORD *et al.* (36) in 1936 and used by most investigators in smoke studies after that date.

[§] Subsequent to the publication of the PREUSSMANN and STEWART review (282b), DEUTSCH-WENZEL *et al.* (80a) reported that in a skin-painting study with *N'*-nitrosornicotine (NNN), tumors were initiated at the site of application. The specific tumorigenic potency of NNN was estimated to be only 0.8% of that of B[a]P. However no dose response relationship was observed with NNN over a treatment range of 12.5 to 200 µg.

Table 6. Polycyclic aromatic hydrocarbons identified in tobacco smoke

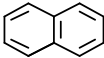
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a	
<i>BICYCLIC: Benzenoid structures</i>				
1	Naphthalene 	[C ₁₀ H ₈] [128]	91-20-3	8, 13–15, 20, 29, 30, 32, 33, 50, 57, 65, 71, 72a, 81, 93, 95, 97, 102, 103, 113, 114, 124, 126–128, 135, 137, 138, 140, 150, 155, 159, 180, 183, 185, 192, 198, 204, 209, 229, 231, 234a, 237, 255, 257, 263, 265, 278, 280, 283, 292, 293, 302, 308, 309, 315, 317, 319, 320, 323, 324, 326, 327, 329, 332, 334, 336, 338, 341, 342, 357, 360, 361, 365, 370, 371–378, 382, 387, 392, 393, 395, 398, 400–402, 407, 415–418, 420–422, 423, 425, 432, 440, 451, 452, 477, 500, 504, 515, 520, 527, 530
2	Naphthalene, alkyl-			323, 370, 372–377, 500, 504
3	Naphthalene, diethyl-	[C ₁₄ H ₁₆] [184]	31831-35-3	7
4	Naphthalene, dihydro-	[C ₁₀ H ₁₀] [130]	29828-28-2	234a, 475
5–7 ^b	Naphthalene, dihydrodimethyl-	[C ₁₂ H ₁₄] [158]	72692-88-7	126, 234a, 263, 392
8–14 ^b	Naphthalene, dihydromethyl-	[C ₁₁ H ₁₂] [144]	39292-53-0	124, 126, 263, 392
15	Naphthalene, 1,2-dihydro-3-methyl-	[C ₁₁ H ₁₂] [144]	2717-44-4	234a, 475
16	Naphthalene, 1,2-dihydro-4-methyl-	[C ₁₁ H ₁₂] [144]	4373-13-1	128, 317, 323, 329, 332, 338
17	Naphthalene, 1,2-dihydro-5-methyl-3-(1-methylethenyl)-	[C ₁₄ H ₁₆] [184]	67494-22-8	79, 464
18	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	[C ₁₃ H ₁₆] [172]	30364-38-6	8, 234a, 342
19	Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	[C ₁₃ H ₁₆] [172]	4506-36-9	126, 234a, 264, 392
A ^c	Naphthalene, dimethyl-	[C ₁₂ H ₁₂] [156]	28804-88-8	124, 126, 135, 234a, 257, 382, 387, 400
20	Naphthalene, 1,2-dimethyl-	[C ₁₂ H ₁₂] [156]	573-98-8	8, 95, 234a, 263, 265, 398, 416, 420
21	Naphthalene, 1,3-dimethyl-	[C ₁₂ H ₁₂] [156]	575-41-7	8, 95, 234a, 263, 265, 392, 398, 400–402, 416, 420–422
22	Naphthalene, 1,4-dimethyl-	[C ₁₂ H ₁₂] [156]	571-58-4	8, 95, 234a, 265, 398, 400–402, 416, 420–422
23	Naphthalene, 1,5-dimethyl-	[C ₁₂ H ₁₂] [156]	571-61-9	8, 95, 234a, 265, 398, 400–402, 416, 420–422
24	Naphthalene, 1,6-dimethyl-	[C ₁₂ H ₁₂] [156]	575-43-9	8, 65, 95, 97, 126, 128, 134, 135, 183, 234a, 255, 263, 265, 319, 323, 338, 342, 392, 398, 400–402, 416, 420–422, 425
25	Naphthalene, 1,7-dimethyl-	[C ₁₂ H ₁₂] [156]	575-37-1	8, 95, 234a, 263, 265, 400–402, 416, 420–422
26	Naphthalene, 1,8-dimethyl-	[C ₁₂ H ₁₂] [156]	569-41-5	8, 32, 65, 95, 97, 234a, 265, 278, 323, 338, 342, 365, 392, 398, 400–402, 416, 420–422, 423, 425
27	Naphthalene, 2,3-dimethyl-	[C ₁₂ H ₁₂] [156]	581-40-8	8, 95, 234a, 265, 392, 398, 400–402, 416, 420–422
28	Naphthalene, 2,6-dimethyl-	[C ₁₂ H ₁₂] [156]	581-42-0	8, 65, 97, 183, 234a, 255, 323, 338, 342, 392, 398, 400–402, 416, 417, 420–422, 425
29	Naphthalene, 2,7-dimethyl-	[C ₁₂ H ₁₂] [156]	582-16-1	8, 65, 95, 97, 183, 234a, 255, 265, 323, 342, 392, 400–402, 416, 420–422
30	Naphthalene, dimethyl-2-ethenyl-	[C ₁₄ H ₁₄] [182]	71630-68-7	234a, 475
31	Naphthalene, dimethylethyl-	[C ₁₄ H ₁₆] [184]	65319-44-0	234a, 392
32	Naphthalene, 1,4-dimethyl-2-ethyl-	[C ₁₄ H ₁₆] [184]	71607-89-1	264, 392
33	Naphthalene, 1,4-dimethyl-5-ethyl-	[C ₁₄ H ₁₆] [184]	66309-90-8	416, 420
34	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-1,2,3,4-tetrahydro-, (1S-cis)-	[C ₁₅ H ₂₂] [202]	483-77-2	109, 463
35	Naphthalene, dimethyl-2-phenyl-	[C ₁₈ H ₁₆] [232]	71607-60-8	234a, 416, 420
36	Naphthalene, dimethyltetrahydro-	[C ₁₂ H ₁₆] [160]		126, 263, 392
37	Naphthalene, dimethyl-1,2,3,4-tetrahydro-	[C ₁₂ H ₁₆] [160]	51855-29-9 65338-07-0	234a, 264
38	Naphthalene, 1-ethenyl-	[C ₁₂ H ₁₀] [154]	826-74-4 72843-02-8	8, 234a, 398, 400–402, 421, 422
39	Naphthalene, 2-ethenyl-	[C ₁₂ H ₁₀] [154]	827-54-3	8, 234a, 398, 400–402, 416, 420–422
40–41 ^b	Naphthalene, 2-ethenylmethyl-	[C ₁₃ H ₁₂] [168]	64031-89-6	234a, 397, 416, 420
42	Naphthalene, 2-ethenyl-1-methyl-	[C ₁₃ H ₁₂] [168]	35737-86-1	475
A ^d	Naphthalene, ethyl-	[C ₁₂ H ₁₂] [156]	27138-19-8	124, 237, 361
43	Naphthalene, 1-ethyl-	[C ₁₂ H ₁₂] [156]	1127-76-0	8, 95, 175, 234a, 265, 392, 398, 400–402, 416, 420–422
44	Naphthalene, 2-ethyl-	[C ₁₂ H ₁₂] [156]	939-27-5	8, 95, 175, 234a, 263, 265, 392, 398, 400–402, 416, 420–422
45	Naphthalene, ethylmethyl-	[C ₁₃ H ₁₄] [170]	31391-42-1	8, 95, 234a, 265, 416, 420
46	Naphthalene, 1-ethyl-3-methyl-	[C ₁₃ H ₁₄] [170]	17057-94-2	95, 265
47	Naphthalene, 1-ethyl-5-methyl-	[C ₁₃ H ₁₄] [170]	17057-92-0	95, 265
48	Naphthalene, 1-ethyl-6-methyl-	[C ₁₃ H ₁₄] [170]	31032-91-4	95, 234a, 265

Table 6 (cont.)

No.	Polycyclic Aromatic Hydrocarbon		CAS RN	References ^a
<i>BICYCLIC: Benzenoid structures (cont.)</i>				
49	Naphthalene, 1-ethyl-7-methyl-	[C ₁₃ H ₁₄] [170]	31032-92-5	95, 234a, 265
50	Naphthalene, 1-ethyl-8-methyl-	[C ₁₃ H ₁₄] [170]	61886-71-3	95, 234a, 265
51	Naphthalene, 2-ethyl-3-methyl-	[C ₁₃ H ₁₄] [170]	31032-94-7	95, 234a, 265
52	Naphthalene, 2-ethyl-4-methyl-	[C ₁₃ H ₁₄] [170]	17179-41-8	95, 265
53	Naphthalene, 2-ethyl-5-methyl-	[C ₁₃ H ₁₄] [170]	17059-53-9	95, 265
54	Naphthalene, 2-ethyl-6-methyl-	[C ₁₃ H ₁₄] [170]	7372-86-3	95, 234a, 265
55	Naphthalene, 2-ethyl-7-methyl-	[C ₁₃ H ₁₄] [170]	17059-55-1	95, 126, 234a, 264, 265
56	Naphthalene, hexamethyl-	[C ₁₆ H ₂₀] [212]	77242-78-5	234a, 416, 420
A ^e	Naphthalene, methyl-	[C ₁₁ H ₁₀] [142]	1321-94-4	234a, 237, 377, 378
57	Naphthalene, 1-methyl-	[C ₁₁ H ₁₀] [142]	90-12-0	8, 13, 65, 97, 124, 126, 128, 134, 135, 155, 180, 183, 192, 234a, 255, 257, 263, 265, 308, 317, 319, 323, 329, 332, 334, 336, 338, 341, 342, 361, 382, 387, 392, 393, 398, 400–402, 407, 415, 416, 420–423, 425, 452, 453
58	Naphthalene, 2-methyl-	[C ₁₁ H ₁₀] [142]	91-57-6	8, 13, 65, 69, 97, 113, 114, 124, 126–128, 134, 135, 155, 168, 180, 183, 192, 234a, 255, 257, 263, 265, 278, 317, 319, 323, 329, 332, 334, 336, 338, 341, 342, 361, 365, 382, 387, 392, 393, 398, 400–402, 407, 415–418, 420–423, 425, 452, 453
59	Naphthalene, (1-methylethyl)-	[C ₁₃ H ₁₄] [170]	29253-36-9	8, 234a, 416, 420
60	Naphthalene, methylphenyl-	[C ₁₇ H ₁₄] [218]	52991-56-7	142, 234a
61	Naphthalene, methyl-2-phenyl-	[C ₁₇ H ₁₄] [218]	71607-61-9	234a, 416, 420
62	Naphthalene, methylpropyl-	[C ₁₄ H ₁₆] [184]	34540-66-4	7
63	Naphthalene, 1-(1-methylpropyl)-	[C ₁₄ H ₁₆] [184]	1680-58-6	7, 95, 234a, 263, 264
64	Naphthalene, 1-(2-methylpropyl)-	[C ₁₄ H ₁₆] [184]	1669-91-6	95
65–67 ^b	Naphthalene, methyltetrahydro-	[C ₁₁ H ₁₄] [146]	71607-57-3	263, 392
68	Naphthalene, methyl-1,2,3,4-tetrahydro-	[C ₁₁ H ₁₄] [146]	31291-71-1	168, 234a
69	Naphthalene, 1-methyl-1,2,3,4-tetrahydro-	[C ₁₁ H ₁₄] [146]	1559-81-5	475
70	Naphthalene, 2-methyl-1,2,3,4-tetrahydro-	[C ₁₁ H ₁₄] [146]	3877-19-8	234a, 261
71	Naphthalene, 5-methyl-1,2,3,4-tetrahydro-	[C ₁₁ H ₁₄] [146]	2809-64-5	7
72	Naphthalene, 6-methyl-1,2,3,4-tetrahydro-	[C ₁₁ H ₁₄] [146]	1680-51-9	1, 7, 260, 261, 400–422
73	Naphthalene, pentamethyl-	[C ₁₅ H ₁₈] [198]	56908-81-7	8, 234a, 416, 420
74	Naphthalene, 1-phenyl-	[C ₁₆ H ₁₂] [204]	605-02-7	1, 234a, 332
75	Naphthalene, 2-phenyl-	[C ₁₆ H ₁₂] [204]	612-94-2	22, 234a, 317, 323, 329, 334, 338, 388, 416, 420, 439
A ^f	Naphthalene, 2-phenyl-, monomethyl-	[C ₁₇ H ₁₄] [218]	71697-04-6	475
76	Naphthalene, 2-phenyl-, monomethyl-	[C ₁₇ H ₁₄] [218]	27378-74-1	475
77	Naphthalene, 1-propyl-	[C ₁₃ H ₁₄] [170]	2765-18-6	95, 234a
78	Naphthalene, 2-propyl-	[C ₁₃ H ₁₄] [170]	2027-19-2	95, 234a
79–81 ^b	Naphthalene, tetrahydrotrimethyl-	[C ₁₃ H ₁₈] [174]	121414-18-4	126, 392
82	Naphthalene, 1,2,3,4-tetrahydro-	[C ₁₀ H ₁₂] [132]	119-64-2	7, 134, 135, 180, 261, 342
83	Naphthalene, 1,2,3,4-tetrahydrotrimethyl-	[C ₁₃ H ₁₈] [174]	72843-02-8	475
84	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	[C ₁₃ H ₁₈] [174]	475-03-6	8, 94, 234a, 263, 342, 392, 407, 425
85–87 ^b	Naphthalene, tetramethyl-	[C ₁₄ H ₁₆] [184]	28652-74-6	7, 126, 234a, 257, 263, 264, 400, 416, 420–422
88–92 ^b	Naphthalene, trimethyl-	[C ₁₃ H ₁₄] [170]	28652-77-9	7, 95, 124, 126, 257, 263, 264, 382, 387, 400–402, 416, 420–422
93 ^g	Naphthalene, trimethyl-	[C ₁₃ H ₁₄] [170]	26856-35-9	234a, 475
94	Naphthalene, 1,2,4-trimethyl-	[C ₁₃ H ₁₄] [170]	2717-42-2	95, 126, 234a, 264, 265, 392
95	Naphthalene, 1,2,6-trimethyl-	[C ₁₃ H ₁₄] [170]	3031-05-8	95, 265
96	Naphthalene, 1,2,7-trimethyl-	[C ₁₃ H ₁₄] [170]	486-34-0	95, 265
97	Naphthalene, 1,3,5-trimethyl-	[C ₁₃ H ₁₄] [170]	2131-39-7	95, 265
98	Naphthalene, 1,3,6-trimethyl-	[C ₁₃ H ₁₄] [170]	3031-08-1	65, 95, 97, 126, 183, 234a, 255, 265, 323, 338, 342, 392, 425
99	Naphthalene, 1,4,5-trimethyl-	[C ₁₃ H ₁₄] [170]	2131-41-1	234a, 263, 264, 392
100	Naphthalene, 1,4,6-trimethyl-	[C ₁₃ H ₁₄] [170]	2131-42-2	95, 265
101	Naphthalene, 1,6,7-trimethyl-	[C ₁₃ H ₁₄] [170]	2245-38-7	95, 128, 234a
102	Naphthalene, 2,3,6-trimethyl-	[C ₁₃ H ₁₄] [170]	829-26-5	95, 234a, 265, 417
103	1,1'-Binaphthylene	[C ₂₀ H ₁₄] [254]	604-53-5	234a, 303, 475

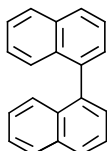


Table 6 (cont.)

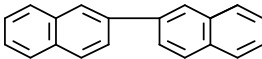
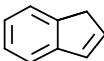
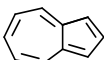
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>BICYCLIC: Benzenoid structures (cont.)</i>			
104	1,1'-Binaphthylene, dimethyl-	[C ₂₂ H ₁₈] [282]	71265-39-9 216
105	1,1'-Binaphthylene, ethyl-	[C ₂₂ H ₁₈] [282]	71277-81-1 216
106	1,1'-Binaphthylene, methyl-	[C ₂₁ H ₁₆] [268]	138497-96-8 216, 234a
107	2,2'-Binaphthylene	[C ₂₀ H ₁₄] [254]	612-78-2 13, 177, 323, 342
			
108	2,2'-Binaphthylene, dimethyl-	[C ₂₂ H ₁₈] [282]	71294-43-4 216
109	2,2'-Binaphthylene, ethyl-	[C ₂₂ H ₁₈] [282]	71277-82-2 216
110	2,2'-Binaphthylene, methyl-	[C ₂₁ H ₁₆] [268]	41637-91-6 216
<i>BICYCLIC: Cyclopentanoid-benzenoid structures</i>			
111	1 <i>H</i> -Indene	[C ₉ H ₈] [116]	95-13-6 8, 13, 15, 65, 120, 121, 126, 134, 135, 140, 237, 240, 257, 263, 323, 336a, 342, 365, 372–374, 376, 390, 392, 398, 407, 415, 416, 420–422, 425
			
112	1 <i>H</i> -Indene, diethyl-	[C ₁₃ H ₁₆] [172]	71278-05-2 416, 420
113	1 <i>H</i> -Indene, 2,3-dihydro-	[C ₉ H ₁₀] [118]	496-11-7 134, 135, 175, 180, 260, 261, 390, 392
114	1 <i>H</i> -Indene, 2,3-dihydropdimethyl-	[C ₁₁ H ₁₄] [146]	53563-67-0 237, 257, 260, 261, 392, 474
115	1 <i>H</i> -Indene, 2,3-dihydro-1,2-dimethyl-	[C ₁₁ H ₁₄] [146]	17057-82-8 263, 264, 392
116	1 <i>H</i> -Indene, 2,3-dihydroethyl-	[C ₁₁ H ₁₄] [146]	71278-02-9 260, 261, 264, 392
117	1 <i>H</i> -Indene, 2,3-dihydropmethyl-	[C ₁₀ H ₁₂] [132]	27133-93-3 126, 237, 240, 257, 260, 261, 361
118	1 <i>H</i> -Indene, 2,3-dihydro-1-methyl-	[C ₁₀ H ₁₂] [132]	767-58-8 126, 168, 261
119	1 <i>H</i> -Indene, 2,3-dihydro-2-methyl-	[C ₁₀ H ₁₂] [132]	824-63-5 260, 261
120	1 <i>H</i> -Indene, 2,3-dihydro-4-methyl-	[C ₁₀ H ₁₂] [132]	824-22-6 180
121	1 <i>H</i> -Indene, 2,3-dihydro-5-methyl-	[C ₁₀ H ₁₂] [132]	874-35-1 264, 392
122	1 <i>H</i> -Indene, 2,3-dihydrotrimethyl-	[C ₁₂ H ₁₆] [160]	36541-18-1 257, 264, 392
123	1 <i>H</i> -Indene, dimethyl-	[C ₁₁ H ₁₂] [144]	29348-63-8 8, 237, 257, 392, 400–402, 416, 420–422
124	1 <i>H</i> -Indene, dimethylethyl-	[C ₁₃ H ₁₆] [172]	71278-06-3 8, 416, 420
125	1 <i>H</i> -Indene, 5,6-dimethyl-2-phenyl-	[C ₁₇ H ₁₆] [220]	22
126	1 <i>H</i> -Indene, 2-(3',4'-dimethylphenyl)-	[C ₁₇ H ₁₆] [220]	22
127	1 <i>H</i> -Indene, ethyl-	[C ₁₁ H ₁₂] [144]	58924-35-9 8, 257, 416, 420
128	1 <i>H</i> -Indene, ethylmethyl-	[C ₁₂ H ₁₄] [158]	77227-01-1 416, 420
129	1 <i>H</i> -Indene, ethylpentamethyl-	[C ₁₆ H ₂₂] [214]	71278-07-4 416, 420
130	1 <i>H</i> -Indene, heptamethyl-	[C ₁₆ H ₂₂] [214]	77242-77-4 416, 420
131	1 <i>H</i> -Indene, hexamethyl-	[C ₁₅ H ₂₀] [200]	71278-08-5 416, 420
132–134 ^b	1 <i>H</i> -Indene, methyl-	[C ₁₀ H ₁₀] [130]	29036-25-7 8, 15, 124, 135, 237, 240, 257, 392, 398, 401, 402, 416, 420–422
135	1 <i>H</i> -Indene, 1-methyl-	[C ₁₀ H ₁₀] [130]	767-59-9 126, 400–402, 416, 420–422
136	1 <i>H</i> -Indene, 2-methyl-	[C ₁₀ H ₁₀] [130]	2177-47-1 576, 400-402, 416, 420
137	1 <i>H</i> -Indene, 3-methyl-	[C ₁₀ H ₁₀] [130]	767-60-2 263, 392, 400, 416, 420–422
138	1 <i>H</i> -Indene, 1-methylene-	[C ₁₀ H ₈] [128]	2471-84-3 392
139	2 <i>H</i> -Indene, 2-methylene-	[C ₁₀ H ₈] [128]	6596-86-7 392
140	1 <i>H</i> -Indene, 4-methyl-2-(2'-methylphenyl)-	[C ₁₇ H ₁₆] [220]	22
141	1 <i>H</i> -Indene, 5-methyl-2-(4'-methylphenyl)-	[C ₁₇ H ₁₆] [220]	22
142	1 <i>H</i> -Indene, 6-methyl-2-(4'-methylphenyl)-	[C ₁₇ H ₁₆] [220]	22
143	1 <i>H</i> -Indene, 7-methyl-2-(2'-methylphenyl)-	[C ₁₇ H ₁₆] [220]	22
144	1 <i>H</i> -Indene, 7-(4'-methylphenyl)-	[C ₁₆ H ₁₄] [206]	22
145	1 <i>H</i> -Indene, pentamethyl-	[C ₁₄ H ₁₈] [186]	71278-09-6 416, 420
146	1 <i>H</i> -Indene, phenyl-	[C ₁₅ H ₁₂] [192]	38638-41-4 166, 416, 420
147	1 <i>H</i> -Indene, 2-phenyl-	[C ₁₅ H ₁₂] [192]	4505-48-0 22
148	1 <i>H</i> -Indene, phenyltrimethyl-	[C ₁₈ H ₁₈] [234]	22
149–152 ^b	1 <i>H</i> -Indene, tetramethyl-	[C ₁₃ H ₁₆] [172]	27135-78-0 8, 257, 416, 420
153–155 ^b	1 <i>H</i> -Indene, trimethyl-	[C ₁₂ H ₁₄] [158]	60826-61-1 8, 237, 257, 400-402, 416, 420–422
156	Azulene	[C ₁₀ H ₈] [128]	275-51-4 97, 113, 114, 150, 173, 194, 195, 221, 227, 228, 231, 235, 278, 283, 323, 338, 407, 425
			

Table 6 (cont.)

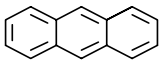
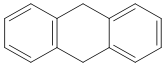
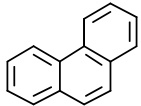
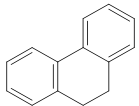
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TRICYCLIC: Benzenoid structures</i>			
157	Anthracene 	[C ₁₄ H ₁₀] [178]	120-12-7 1, 4, 5, 8, 11, 13, 22, 29, 30, 32–34, 43, 44, 50, 51a, 57, 61, 67-69, 71, 72a, 74, 76, 81, 93, 96, 97, 100, 102, 103, 111, 114, 124, 128, 133a, 135, 137, 138, 150, 159, 174, 178, 185, 187, 191, 198, 209, 219, 221-223, 225, 227, 231, 236, 239a, 241, 249, 251–253, 263, 273, 274, 278, 280, 282, 283, 287, 289, 302, 308–310, 315, 317, 319, 320, 323, 326, 329-336, 336a, 338, 341, 342, 345, 347, 357, 361, 363-368, 370, 372-378, 388, 392, 395, 398, 400–402, 417, 418, 421–425, 433, 434, 440, 445–447, 474, 477, 479, 483, 484, 494, 511, 515, 517-520, 524, 526, 529, 530
158	Anthracene, alkyl-		69, 100, 229, 273, 278, 323, 342, 372–374, 376, 479, 520
159	Anthracene, 9,10-dihydro- 	[C ₁₄ H ₁₂] [180]	613-31-0 5, 97, 280, 323, 338, 388, 425
160–162 ^b	Anthracene, dimethyl-	[C ₁₆ H ₁₄] [206]	29063-00-1 368, 388, 400–402, 416, 420–422, 440, 530
163	Anthracene, 9,10-dimethyl-	[C ₁₆ H ₁₄] [206]	781-43-1 30, 336, 353, 388, 529, 530
164	Anthracene, ethyl-	[C ₁₆ H ₁₄] [206]	41637-86-9 142, 263
165	Anthracene, 9-ethyl-	[C ₁₆ H ₁₄] [206]	605-83-4 475
166	Anthracene, ethylmethyl-	[C ₁₇ H ₁₆] [220]	71265-29-7 216
167	Anthracene, 1-methyl-	[C ₁₅ H ₁₂] [192]	610-48-0 400–402, 416, 420–422, 440
168	Anthracene, 2-methyl-	[C ₁₅ H ₁₂] [192]	613-12-7 22, 29, 69, 97, 138, 278, 323, 338, 342, 365, 392, 398, 400–402, 416, 420–422, 423–425, 440
169	Anthracene, 9-methyl-	[C ₁₅ H ₁₂] [192]	779-02-2 5, 29, 30, 72a, 138, 302, 317, 323, 329, 332, 334, 338, 342, 388, 398, 400–402, 416, 420–422, 423–425, 440, 530
170	Anthracene, propyl-	[C ₁₇ H ₁₆] [220]	71265-30-0 216
171–172 ^b	Anthracene, trimethyl-	[C ₁₇ H ₁₆] [220]	27358-28-7 216, 400–402, 416, 420–422, 530
173	Phenanthrene 	[C ₁₄ H ₁₀] [178]	85-01-8 1, 5, 8, 11, 13, 20, 29, 30, 32, 33, 44, 51a, 57, 65, 68, 69, 71, 72a, 81, 96, 97, 100, 102, 103, 113, 114, 116, 117, 124, 126, 127, 133a, 135, 138, 150, 159, 185, 187, 192, 196, 198, 204, 209, 221, 231, 238, 239a, 249, 255, 257, 263, 267, 270, 274, 278, 280–283, 285, 288, 289, 292, 293, 302, 308–310, 315, 317, 319, 320, 323, 326, 329, 334, 336, 336a, 338, 341, 342, 345, 346, 348, 357, 361, 364-366, 368, 370, 372–378, 388, 392, 398, 400–402, 410, 415, 417, 418, 421–423, 425, 434, 440, 474, 477, 479, 484, 494, 515, 520, 529, 530
174	Phenanthrene, alkyl-		13, 51a, 100, 342, 372-374, 376, 479
175	Phenanthrene, dihydro-	[C ₁₄ H ₁₂] [180]	26856-35-9 198, 342
176	Phenanthrene, 9,10-dihydro- 	[C ₁₄ H ₁₄] [182]	776-35-2 126, 342
177	Phenanthrene, dihydromethylene-	[C ₁₆ H ₁₂] [204]	71607-56-2 475
A ^h	Phenanthrene, dimethyl-	[C ₁₆ H ₁₄] [206]	29062-98-4 32, 51a, 317, 323, 329, 332, 334, 368, 388, 400–402, 419, 421, 422, 529
178	Phenanthrene, 1,2-dimethyl-	[C ₁₆ H ₁₄] [206]	20291-72-9 21, 128
179	Phenanthrene, 1,4-dimethyl-	[C ₁₆ H ₁₄] [206]	22349-59-3 174
180	Phenanthrene, 1,6-dimethyl-	[C ₁₆ H ₁₄] [206]	20291-74-1 21
181	Phenanthrene, 1,7-dimethyl-	[C ₁₆ H ₁₄] [206]	483-87-4 21
182	Phenanthrene, 1,8-dimethyl-	[C ₁₆ H ₁₄] [206]	7372-87-4 1, 182, 278, 323, 338, 342, 425
183	Phenanthrene, 2,5-dimethyl-	[C ₁₆ H ₁₄] [206]	3674-66-6 21, 365
184	Phenanthrene, 2,6-dimethyl-	[C ₁₆ H ₁₄] [206]	17980-16-4 21
185	Phenanthrene, 2,7-dimethyl-	[C ₁₆ H ₁₄] [206]	1576-69-8 4, 5, 388
186	Phenanthrene, 3,6-dimethyl-	[C ₁₆ H ₁₄] [206]	1576-67-6 196, 338
187	Phenanthrene, 4,5-dimethyl-	[C ₁₆ H ₁₄] [206]	3674-69-9 419, 421, 422
188	Phenanthrene, dimethylethyl-	[C ₁₈ H ₁₈] [234]	71607-65-3 475
189	Phenanthrene, ethyl-	[C ₁₆ H ₁₄] [206]	30997-38-7 475

Table 6 (cont.)

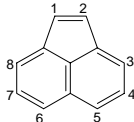
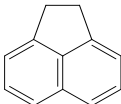
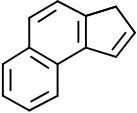
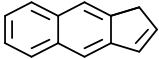
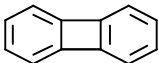
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TRICYCLIC: Benzenoid structures (cont.)</i>			
190	Phenanthrene, ethylmethyl-	[C ₁₇ H ₁₆] [220]	71607-66-4 475
191	Phenanthrene, hexamethyl-	[C ₂₀ H ₂₂] [262]	71607-67-5 475
A ⁱ	Phenanthrene, methyl-	[C ₁₅ H ₁₂] [192]	31711-53-2 8, 128, 198, 323, 342, 361, 368, 377, 378, 388, 392, 417, 440, 474
192	Phenanthrene, 1-methyl-	[C ₁₅ H ₁₂] [192]	832-69-9 5, 174, 263, 361, 388, 392, 398, 400–402, 416, 420–422, 425
193	Phenanthrene, 2-methyl-	[C ₁₅ H ₁₂] [192]	2531-84-2 5, 263, 392, 398, 400, 416, 420–422
194	Phenanthrene, 3-methyl-	[C ₁₅ H ₁₂] [192]	832-71-3 4, 5, 263, 388, 398, 400, 416, 420–422
195	Phenanthrene, 4-methyl-	[C ₁₅ H ₁₂] [192]	832-64-4 21, 398, 400–402, 421, 422
196	Phenanthrene, 9-methyl-	[C ₁₅ H ₁₂] [192]	883-20-5 1, 31, 32, 249, 278, 317, 323, 329, 332, 334, 338, 365, 398, 400–402, 416, 420–422, 425
197	Phenanthrene, 1-methyl-5-(1-methylethyl)-	[C ₁₈ H ₁₈] [234]	475
198	Phenanthrene, pentamethyl-	[C ₁₉ H ₂₀] [248]	71607-68-6 216, 416, 420
199	Phenanthrene, propyl-	[C ₁₇ H ₁₆] [220]	71607-69-7 216
200–204 ^b	Phenanthrene, tetramethyl-	[C ₁₇ H ₁₆] [234]	71607-70-0 336, 416, 420, 529
205–207 ^b	Phenanthrene, trimethyl-	[C ₁₇ H ₁₆] [220]	30232-26-9 400–402, 416, 420–422
<i>TRICYCLIC: Cyclopentanoid-benzenoid structures</i>			
208	Acenaphthylene	[C ₁₂ H ₈] [152]	208-96-8 3, 8, 13, 29, 32, 33, 43, 44, 67–70, 81, 97, 113, 114, 124, 126, 127, 134, 135, 137, 150, 155, 174, 185, 198, 209, 221–223, 227–229, 231, 257, 278, 280, 308, 313, 315, 317, 323, 329, 334, 336, 338, 341, 342, 357, 361, 365, 370, 372–374, 376, 379, 392, 398, 400–402, 415, 416, 420–422, 423, 425, 434, 447, 500, 518, 519, 520, 530
			
209	Acenaphthylene, 1,2-dihydro-	[C ₁₂ H ₁₀] [154]	83-32-9 8, 29, 32, 33, 50, 65, 72a, 97, 113, 114, 134, 135, 185, 197, 198, 209, 257, 263, 278, 280, 315, 317, 323, 329, 332, 334, 336, 338, 341, 342, 357, 365, 376, 379, 388, 392, 398, 400–402, 416, 420–422, 425, 524, 530
			
210	Acenaphthylene, 1,2-dihydropdimethyl-	[C ₁₄ H ₁₄] [182]	60684-29-9 400–402, 416, 420–422
211	Acenaphthylene, 1,2-dihydropmethyl-	[C ₁₃ H ₁₂] [168]	36541-21-6 379, 400–402, 416, 420–422
212	Acenaphthylene, 1,2-dihydropmethyl-	[C ₁₆ H ₁₆] [210]	60826-72-4 400–402, 416, 420–422
213–214 ^b	Acenaphthylene, 1,2-dihydroptrimethyl-	[C ₁₅ H ₁₆] [196]	60826-69-9 400–402, 420–422
215–216 ^b	Acenaphthylene, dimethyl-	[C ₁₄ H ₁₂] [180]	60826-68-8 8, 216, 400–402, 416, 420–422
217	Acenaphthylene, 1,3-dimethyl-	[C ₁₄ H ₁₂] [180]	19346-00-0 304
218	Acenaphthylene, diphenyl-	[C ₂₄ H ₁₆] [304]	58546-40-6 216
219–220 ^b	Acenaphthylene, methyl-	[C ₁₃ H ₁₀] [166]	58548-38-2 8, 257, 398, 400–402, 416, 420–422
221	Acenaphthylene, 1-methyl-	[C ₁₃ H ₁₀] [166]	19345-99-4 397, 400, 421, 422
222	Acenaphthylene, 3-methyl-	[C ₁₃ H ₁₀] [166]	19345-94-9 397, 399
223	Acenaphthylene, 4-methyl-	[C ₁₃ H ₁₀] [166]	19345-97-2 99
224	Acenaphthylene, 5-methyl-	[C ₁₃ H ₁₀] [166]	19345-91-6 99
225–226 ^b	Acenaphthylene, tetramethyl-	[C ₁₆ H ₁₆] [208]	60826-73-5 400–402, 416, 420–422
227–228 ^b	Acenaphthylene, trimethyl-	[C ₁₅ H ₁₄] [194]	60826-70-2 8, 400–402, 416, 420–422
229	1 <i>H</i> -Benz[e]indene	[C ₁₃ H ₁₀] [166]	232-54-2 397
			
230	1 <i>H</i> -Benz[e]indene, dimethyl-	[C ₁₅ H ₁₄] [194]	416, 420
231	1 <i>H</i> -Benz[e]indene, methyl-	[C ₁₄ H ₁₂] [180]	64031-90-9 397
232	1 <i>H</i> -Benz[f]indene	[C ₁₃ H ₁₀] [166]	268-40-6 398, 400–402, 421, 422
			
233	1 <i>H</i> -Benz[f]indene, dimethyl-	[C ₁₅ H ₁₄] [194]	60826-71-3 400–402, 416, 420–422
234	1 <i>H</i> -Benz[f]indene, ethylmethyl-	[C ₁₆ H ₁₆] [208]	71265-34-4 416, 420
235–237 ^b	1 <i>H</i> -Benz[f]indene, methyl-	[C ₁₄ H ₁₂] [180]	60826-63-3 400–402, 419, 421, 422
238	Biphenylene	[C ₁₂ H ₈] [152]	259-79-0 475
			

Table 6 (cont.)

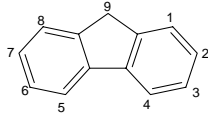
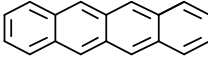
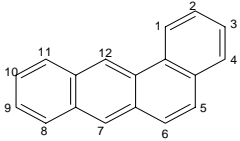
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TRICYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
239	9 <i>H</i> -Fluorene 	[C ₁₃ H ₁₀] [166]	86-73-7 1, 5, 8, 13, 22, 29, 32, 33, 51a, 57, 72a, 97, 113, 114, 124, 126–128, 135, 138, 157a, 159, 174, 185, 198, 238, 239, 239a, 249, 257, 263, 267, 278, 280, 282, 294, 302, 317, 323, 324, 329, 332, 334, 336, 338, 342, 357, 361, 365, 370, 372–374, 376–378, 383, 388, 391, 392, 398, 400–402, 415–417, 420–422, 423, 425, 445, 446, 515, 527, 530
240–244 ^b	9 <i>H</i> -Fluorene, dimethyl-	[C ₁₅ H ₁₄] [194]	30582-01-5 22, 294, 392, 400–402, 416, 420–422
245	9 <i>H</i> -Fluorene, ? ,9-dimethyl-	[C ₁₅ H ₁₄] [194]	416, 420
246	9 <i>H</i> -Fluorene, 1,9-dimethyl-	[C ₁₅ H ₁₄] [194]	17057-98-6 157a, 263, 295, 392
247	9 <i>H</i> -Fluorene, 2,3-dimethyl-	[C ₁₅ H ₁₄] [194]	4612-63-9 157a, 263, 295
248	9 <i>H</i> -Fluorene, 9,9-dimethyl-	[C ₁₅ H ₁₄] [194]	4569-45-3 157a, 263
249	9 <i>H</i> -Fluorene, dimethylethyl-	[C ₁₇ H ₁₈] [222]	71278-00-7 416, 420
250–251 ^b	9 <i>H</i> -Fluorene, ethyl-	[C ₁₅ H ₁₄] [194]	65319-49-5 416, 420
252	9 <i>H</i> -Fluorene, 2-ethyl-	[C ₁₅ H ₁₄] [194]	1207-20-1 157a, 263
253	9 <i>H</i> -Fluorene, 9-ethyl-	[C ₁₅ H ₁₄] [194]	2294-82-8 416, 420
254–255 ^b	9 <i>H</i> -Fluorene, ethylmethyl-	[C ₁₆ H ₁₆] [208]	71278-01-8 416, 420
A ^j	9 <i>H</i> -Fluorene, methyl-	[C ₁₄ H ₁₂] [180]	26914-17-0 22, 51a, 124, 239, 388
256	9 <i>H</i> -Fluorene, 1-methyl-	[C ₁₄ H ₁₂] [180]	1730-37-6 5, 8, 22, 97, 157a, 263, 278, 294, 323, 365, 398, 400–402, 416, 420–422, 425, 455
257	9 <i>H</i> -Fluorene, 2-methyl-	[C ₁₄ H ₁₂] [180]	1430-97-3 8, 22, 126, 128, 157a, 263, 294, 388, 391, 392, 398, 400–402, 416, 420–422;
258	9 <i>H</i> -Fluorene, 3-methyl-	[C ₁₄ H ₁₂] [180]	2523-39-9 8, 22, 157a, 294, 392, 400–402, 416, 420–422,
259	9 <i>H</i> -Fluorene, 4-methyl-	[C ₁₄ H ₁₂] [180]	1556-99-6 8, 22, 128, 157a, 263, 294, 365, 392, 400–402, 416, 420–422
260	9 <i>H</i> -Fluorene, 9-methyl-	[C ₁₄ H ₁₂] [180]	2523-37-7 8, 22, 32, 97, 157a, 249, 263, 278, 323, 338, 365, 398, 401, 402, 416, 420–422, 425, 455
261	9 <i>H</i> -Fluorene, 9-methylene-	[C ₁₄ H ₁₀] [178]	4425-82-5 159, 295
262	9 <i>H</i> -Fluorene, tetramethyl-	[C ₁₇ H ₁₈] [222]	63372-50-9 416, 420
263	9 <i>H</i> -Fluorene, trimethyl-	[C ₁₆ H ₁₆] [208]	30582-02-6 416, 420
<i>TETRACYCLIC: Benzenoid structures</i>			
264	Naphthacene 	[C ₁₈ H ₁₂] [228]	92-24-0 50, 65, 71, 97, 206, 239, 281, 302, 323, 425, 530
265	Benzenanthracene, methyl-	[C ₁₉ H ₁₄] [242]	63194-18-3 416, 420
266	Benz[<i>a</i>]anthracene 	[C ₁₈ H ₁₂] [228]	56-55-3 1, 8, 11, 13, 19, 20, 29, 30, 32–35, 50, 51a, 57, 64, 71, 72a, 89, 96, 97, 100, 102, 103, 106, 113, 114, 116–119, 122, 127, 128, 131, 131a, 133a, 138, 152–157, 160, 162, 163, 165, 167, 174, 182, 185, 187, 191, 192, 198, 204, 219, 222, 223, 227, 230, 238, 239a, 249, 268, 273, 278, 279, 280, 282, 283, 286, 288, 292, 293, 297, 299–302, 308–310, 315, 317, 319, 320, 323, 325, 326, 328–332, 334, 336, 338, 341, 342, 357, 365, 368, 377, 378, 383, 398, 400–402, 414, 417, 419–422, 424–426, 432, 436, 439, 440, 441, 443, 444, 447–453, 474, 477, 484, 490, 491, 494, 496, 497, 500, 501, 503, 509, 510, 520, 530, 496
267	Benz[<i>a</i>]anthracene, alkyl-		496
268–269 ^b	Benz[<i>a</i>]anthracene, dimethyl-	[C ₂₀ H ₁₆] [256]	43178-07-0 71, 341, 400–402, 419–422, 529, 530
270	Benz[<i>a</i>]anthracene, 7,12-dimethyl-	[C ₂₀ H ₁₆] [256]	57-97-6 30, 71, 72a, 97, 196, 198, 204, 278, 280, 282, 283, 320, 323, 336, 338, 342, 356, 365, 409–412, 423, 424, 440, 461, 494, 499, 500, 504, 507, 510, 529, 530
271	Benz[<i>a</i>]anthracene, ethyl-	[C ₂₀ H ₁₆] [256]	31632-62-9 71, 216, 336, 529
272	Benz[<i>a</i>]anthracene, ethylmethyl-	[C ₂₁ H ₁₈] [270]	71265-32-2 475
273	Benz[<i>a</i>]anthracene, methyl-	[C ₁₉ H ₁₄] [242]	43178-22-9 239, 398, 401, 402, 419, 421, 422
274	Benz[<i>a</i>]anthracene, 1-methyl-	[C ₁₉ H ₁₄] [242]	2498-77-3 71, 216, 400; 419–422, 530
275	Benz[<i>a</i>]anthracene, 2-methyl-	[C ₁₉ H ₁₄] [242]	2498-76-2 56, 71, 530
276	Benz[<i>a</i>]anthracene, 3-methyl-	[C ₁₉ H ₁₄] [242]	2498-75-1 71, 97, 216, 278, 530
277	Benz[<i>a</i>]anthracene, 4-methyl-	[C ₁₉ H ₁₄] [242]	316-49-4 71, 216, 530

Table 6 (cont.)

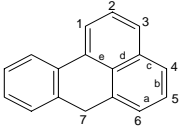
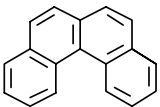
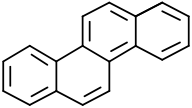
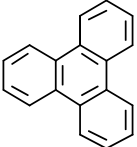
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TETRACYCLIC: Benzenoid structures (cont.)</i>			
278	Benz[<i>a</i>]anthracene, 5-methyl-	[C ₁₉ H ₁₄] [242]	2319-96-2 32, 71, 97, 249, 286, 317, 323, 329, 332, 334, 336, 338, 365, 425, 530
279	Benz[<i>a</i>]anthracene, 6-methyl-	[C ₁₉ H ₁₄] [242]	316-14-3 71, 216; 336, 529
280	Benz[<i>a</i>]anthracene, 8-methyl-	[C ₁₉ H ₁₄] [242]	2381-31-9 71, 216; 336, 529, 530
281	Benz[<i>a</i>]anthracene, 9-methyl-	[C ₁₉ H ₁₄] [242]	2381-16-0 71, 204, 216, 529, 530
282	Benz[<i>a</i>]anthracene, 10-methyl-	[C ₁₉ H ₁₄] [242]	2381-15-9 71, 216, 529, 530
283	Benz[<i>a</i>]anthracene, 12-methyl-	[C ₁₉ H ₁₄] [242]	2422-79-9 71, 475, 365, 529, 530
284	Benz[<i>a</i>]anthracene, methylene-	[C ₁₉ H ₁₂] [240]	419
285	Benz[<i>a</i>]anthracene, propyl-	[C ₂₁ H ₁₈] [270]	71265-33-3 216, 529
286	Benz[<i>a</i>]anthracene, tetramethyl-	[C ₂₂ H ₂₀] [284]	71, 416, 420, 529
287–288 ^b	Benz[<i>a</i>]anthracene, trimethyl-	[C ₂₁ H ₁₈] [270]	60826-78-0 71, 216, 336, 400–402, 416, 420–422, 529, 530
289	7 <i>H</i> -Benz[<i>de</i>]anthracene	[C ₁₇ H ₁₂] [216]	199-94-0 24a
			
290	Benzo[<i>c</i>]phenanthrene	[C ₁₈ H ₁₂] [228]	195-19-7 37, 71, 97, 127, 133a, 150, 231, 165, 174, 278, 283, 317, 320, 323, 329, 332, 334, 336, 338, 365, 388, 416, 419, 420, 423, 424, 445, 446, 448–456, 459, 474, 500, 509, 510, 520, 529, 530
			
291	Benzo[<i>c</i>]phenanthrene, methyl-	[C ₁₉ H ₁₄] [242]	78328-47-9 38, 71, 336, 529, 530
292	Chrysene	[C ₁₈ H ₁₂] [228]	218-01-9 1, 8, 11, 13, 29, 30, 37, 51a, 57, 71, 81, 96, 97, 100, 106, 131, 131a, 133a, 137, 138, 141, 146, 150, 152, 153, 156, 160, 162, 163, 165, 167, 174, 185, 187, 191, 198, 201, 204, 209, 230, 231, 238, 268, 273, 278, 280, 282, 283, 286, 300, 302, 308–311, 314, 315, 317, 319, 320, 323, 324, 326, 327, 329–334, 336, 338, 342, 357, 358, 365, 368, 370, 377, 378, 383, 388, 396, 398, 400–402, 417, 419, 421–426, 434, 438–440, 448–453, 459, 461, 467, 474, 477, 479, 484, 490, 491, 496, 498, 500, 502, 503, 519, 520, 529, 530
			
293	Chrysene, alkyl-		11, 13, 100, 97, 162, 163, 273, 278, 317, 327, 329, 332, 342, 479, 484, 490–492, 496, 500
294	Chrysene, dimethyl-	[C ₂₀ H ₁₆] [256]	41637-92-7 1, 11, 97, 278, 283, 286, 323, 338, 365, 400–402, 419–422, 425, 529, 530
295	Chrysene, ethyl-	[C ₂₀ H ₁₆] [256]	71277-86-6 166, 379
296	Chrysene, ethylmethyl-	[C ₂₁ H ₁₈] [270]	71277-87-7 216
A ^k	Chrysene, methyl-	[C ₁₉ H ₁₄] [242]	41637-90-5 11, 163, 239, 317, 329, 332, 334, 342, 368, 398, 459, 474
297	Chrysene, 1-methyl-	[C ₁₉ H ₁₄] [242]	3351-28-8 1, 97, 131, 146, 174, 278, 323, 338, 400–402, 419–422, 425, 448–453, 459, 530
298	Chrysene, 2-methyl-	[C ₁₉ H ₁₄] [242]	3351-32-4 131, 146, 166, 174, 400–402, 419–422, 448–450, 451–453, 529, 530
299	Chrysene, 3-methyl-	[C ₁₉ H ₁₄] [242]	3351-31-3 29, 131, 146, 166, 174, 400–402, 419–422, 448–450, 451–453, 529, 530
300	Chrysene, 4-methyl-	[C ₁₉ H ₁₄] [242]	3351-30-2 166, 174, 400–402, 419–422, 529, 530
301	Chrysene, 5-methyl-	[C ₁₉ H ₁₄] [242]	3697-24-3 19, 106, 145, 146, 152–157, 160, 166, 167, 174, 268, 319, 320, 322, 326, 336, 357, 400–402, 414, 414a, 448–453, 500, 509, 529, 530
302	Chrysene, 6-methyl-	[C ₁₉ H ₁₄] [242]	1705-85-7 29, 131, 146, 166, 174, 400, 419–422, 448–453, 529, 530
303	Chrysene, pentamethyl-	[C ₂₃ H ₂₂] [298]	71277-88-8 216; 416, 420
304	Chrysene, propyl-	[C ₂₁ H ₁₈] [270]	71277-89-9 216
305	Chrysene, tetramethyl-	[C ₂₂ H ₂₀] [284]	71277-90-2 416, 420
306	Chrysene, trimethyl-	[C ₂₁ H ₁₈] [270]	60826-77-9 400–402, 416, 420–422
307	Triphenylene	[C ₁₈ H ₁₂] [228]	217-59-4 8, 71, 174, 131a, 133a, 150, 177, 231, 283, 323, 398, 400–402, 419, 421, 422, 423, 424, 440, 496, 529, 530
			

Table 6 (cont.)

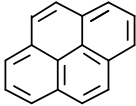
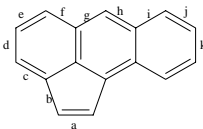
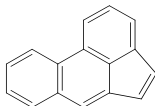
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TETRACYCLIC: Benzenoid structures (cont.)</i>			
308	Triphenylene, dimethyl-	[C ₂₀ H ₁₆] [256]	60826-76-8 400-402, 419-422
309	Triphenylene, methyl-	[C ₁₉ H ₁₄] [242]	41637-89-2 400-402, 419, 421, 422, 530
310	Triphenylene, trimethyl-	[C ₂₁ H ₁₈] [270]	60826-79-1 400-402, 421, 422
311	Pyrene	[C ₁₆ H ₁₀] [202]	129-00-0 1, 4, 5, 8, 11, 13, 20, 22, 29, 30, 32–35, 43, 44–46, 51a, 57, 61, 67–69, 71, 72a, 76, 81, 93, 96, 97, 100, 113, 114, 127, 128, 131, 131a, 133a, 137, 138, 141, 150, 155, 162, 163, 174, 185, 187, 192, 198, 200, 209, 219–223, 227, 229–231, 234a, 236, 239a, 241, 246, 249, 251–253, 271, 273, 274, 278–280, 282, 283, 285, 287–289, 302, 308–311, 314, 315, 317, 319, 320, 323, 326, 327, 329, 332–334, 336, 338, 341, 342, 357, 363–366, 368, 370, 372–374, 376–378, 388, 396, 398, 400–402, 410, 411, 418, 419, 421–425, 427, 433, 434, 439, 440, 445–456, 459, 467, 474, 477, 479, 484, 490, 491, 494, 496, 500, 519, 520, 524, 526, 530
			
312	Pyrene, alkyl-		81, 100, 162, 163, 229, 273, 274, 278, 323, 342, 419, 421, 422, 434, 479, 484, 490, 491, 496, 500
313	Pyrene, 1-butyl-	[C ₂₀ H ₁₈] [258]	35980-18-8 353
314	Pyrene, 1-decyl-	[C ₂₆ H ₃₀] [342]	55682-90-1 353
315	Pyrene, dihydro-	[C ₁₆ H ₁₂] [204]	28779-32-0 198, 200, 234a, 342
316-318 ^b	Pyrene, dimethyl-	[C ₁₈ H ₁₄] [230]	30582-03-7 166, 234a, 368, 398, 400–402, 419–422
319	Pyrene, 1,3-dimethyl-	[C ₁₈ H ₁₄] [230]	64401-21-4 475
320	Pyrene, dimethyl-3,4-dimethylene-	[C ₂₀ H ₁₆] [256]	419
321	Pyrene, 3,4-dimethylene-	[C ₁₈ H ₁₂] [228]	25732-74-5 234a, 397, 400–402, 419, 421, 422
322	Pyrene, 3,4-dimethylenemethyl-	[C ₁₉ H ₁₄] [242]	419
323	Pyrene, ethyl-	[C ₁₈ H ₁₄] [230]	56142-12-2 100, 278, 323
324	Pyrene, 1-ethyl-	[C ₁₈ H ₁₄] [230]	56142-12-2 278, 338, 353
325	Pyrene, ethylmethyl-	[C ₁₉ H ₁₆] [244]	71607-74-4 216
326	Pyrene, hexamethyl-	[C ₂₂ H ₂₂] [286]	71607-75-5 234a, 416, 420
327	Pyrene, 1-hexyl-	[C ₂₂ H ₂₂] [286]	72692-89-8 234a, 353
A ¹	Pyrene, methyl-	[C ₁₇ H ₁₂] [216]	27577-90-8 1, 8, 81, 234a, 287, 317, 323, 329, 332, 342, 377, 378, 434, 440, 448-450, 451-456, 459, 474
328	Pyrene, 1-methyl-	[C ₁₇ H ₁₂] [216]	2381-21-7 32, 69, 97, 113, 114, 128, 138, 234a, 246, 249, 278, 302, 308, 309, 317, 323, 329, 332, 334, 338, 342, 365, 368, 398, 400–402, 419, 421–425, 461, 530
329	Pyrene, 2-methyl-	[C ₁₇ H ₁₂] [216]	3442-78-2 97, 234a, 278, 317, 323, 329, 332, 334, 338, 342, 365, 368, 398, 400–402, 419, 421-425, 455, 459, 520, 521, 530
330	Pyrene, 4-methyl-	[C ₁₇ H ₁₂] [216]	3353-12-6 32, 81, 97, 128, 138, 141, 163, 234a, 246, 249, 278, 280, 317, 323, 329, 332, 334, 338, 342, 365, 368, 398, 400–402, 419, 421–425, 459, 530
331	Pyrene, 1-octyl-	[C ₂₄ H ₂₆] [314]	71608-00-9 353
332–334 ^b	Pyrene, pentamethyl-	[C ₂₁ H ₂₀] [272]	71607-76-6 234a, 416, 420
335	Pyrene, propyl-	[C ₁₉ H ₁₆] [244]	56142-09-7 216
336	Pyrene, 1-tetradecyl-	[C ₃₀ H ₃₈] [398]	71630-71-2 353
337	Pyrene, tetrahydro-	[C ₁₆ H ₁₂] [206]	66161-17-9 200, 201, 342
338–341 ^b	Pyrene, tetramethyl-	[C ₂₀ H ₁₆] [258]	60826-75-7 234a, 400–402, 419–422
342–344 ^b	Pyrene, trimethyl-	[C ₁₉ H ₁₆] [244]	41637-88-1 234a, 216, 400–402, 419–422
<i>TETRACYCLIC: Cyclopentanoid-benzenoid structures</i>			
345	Aceanthrylene	[C ₁₆ H ₁₀] [202]	202-03-9 400–402
			
346	Acephenanthrylene	[C ₁₆ H ₁₀] [202]	201-06-9 174, 368, 398, 400–402, 417, 419
			

Table 6 (cont.)

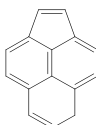
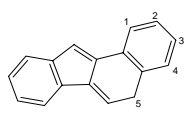
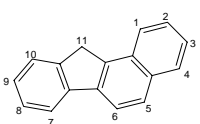
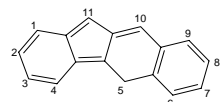
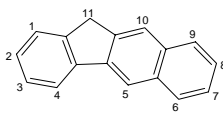
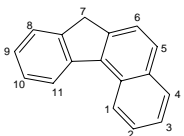
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TETRACYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
347	Acephenanthrylene, 4,5-dihydro-	[C ₁₆ H ₁₂] [204]	6232-48-0 399, 400
348	5 <i>H</i> -Benz[<i>fg</i>]acenaphthylene	[C ₁₅ H ₁₀] [190]	76774-50-0 475
			
349	Benzofluorene, alkyl-		475
350–352 ^b	Benzofluorene, dimethyl-	[C ₁₉ H ₁₆] [244]	7691-50-2 419–422
353–356 ^b	Benzofluorene, methyl-	[C ₁₈ H ₁₄] [230]	60918-47-0 400–402, 419–422
357–358 ^b	Benzofluorene, tetramethyl-	[C ₂₁ H ₂₀] [272]	7691-51-3 416, 420
359	Benzofluorene, trimethyl-	[C ₂₀ H ₁₈] [258]	401, 402
360	Benzo[<i>a</i>]fluorene	[C ₁₇ H ₁₂] [216]	30777-18-5 51a, 131, 133a, 174, 239a, 323, 474
361	5 <i>H</i> -Benzo[<i>a</i>]fluorene	[C ₁₇ H ₁₂] [216]	238-79-9 97, 174, 323, 425
			
362	11 <i>H</i> -Benzo[<i>a</i>]fluorene	[C ₁₇ H ₁₂] [216]	238-84-6 1, 5, 11, 13, 32, 33, 97, 131, 133a, 174, 249, 278, 323, 338, 342, 365, 400–402, 416, 420–422, 424, 425, 454–456, 459, 496, 520
			
363	11 <i>H</i> -Benzo[<i>a</i>]fluorene, dimethyl-	[C ₁₉ H ₁₆] [244]	400, 421, 422
364	11 <i>H</i> -Benzo[<i>a</i>]fluorene, methyl-	[C ₁₈ H ₁₄] [230]	60826-64-4 11, 400–402, 419, 421, 422
365	11 <i>H</i> -Benzo[<i>a</i>]fluorene, 11-methyl-	[C ₁₈ H ₁₄] [230]	71265-25-3 1, 11, 32, 97, 249, 278, 323, 338, 342, 425
366–368 ^b	11 <i>H</i> -Benzo[<i>a</i>]fluorene, trimethyl-	[C ₂₀ H ₁₈] [258]	71607-85-7 400, 416, 420
369	5 <i>H</i> -Benzo[<i>b</i>]fluorene	[C ₁₇ H ₁₂] [216]	243-18-5 97, 131, 133a, 174, 239a, 273, 278, 323, 365, 425 30777-19-6
			
370	11 <i>H</i> -Benzo[<i>b</i>]fluorene	[C ₁₇ H ₁₂] [216]	243-17-4 1, 5, 29, 97, 131, 133a, 163, 174, 278, 338, 342, 401, 402, 419, 421, 422, 424, 425, 484, 496
			
371	11 <i>H</i> -Benzo[<i>b</i>]fluorene, methyl-	[C ₁₈ H ₁₄] [230]	60826-65-5 400-402, 419, 421, 422
372	11 <i>H</i> -Benzo[<i>b</i>]fluorene, 9-methyl-	[C ₁₈ H ₁₄] [230]	419
373	Benzo[<i>c</i>]fluorene, methyl-	[C ₁₈ H ₁₄] [230]	416, 420
374	7 <i>H</i> -Benzo[<i>c</i>]fluorene	[C ₁₇ H ₁₂] [216]	205-12-9 97, 131, 133a, 174, 323, 338, 400–402, 419, 421, 422, 425, 520, 530
			
375	7 <i>H</i> -Benzo[<i>c</i>]fluorene, methyl-	[C ₁₈ H ₁₄] [230]	60826-66-6 400–402, 416, 420–422

Table 6 (cont.)

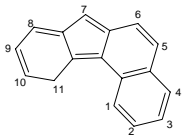
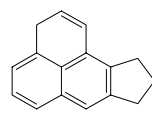
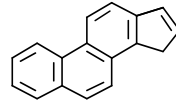
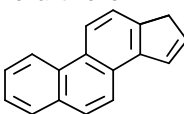
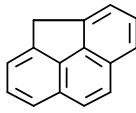
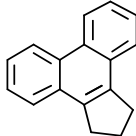
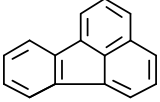
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TETRACYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
376	11 <i>H</i> -Benzo[<i>c</i>]fluorene	[C ₁₇ H ₁₂] [216]	174, 379
			
377	Cyclopenta[<i>a</i>]phenalene	[C ₁₆ H ₁₄] [206]	211-95-0 216
			
378–379 ^b	Cyclopentaphenanthrene	[C ₁₇ H ₁₄] [218]	80455-52-3 398, 400–402, 416, 420–422
380–381 ^b	Cyclopentaphenanthrene, methyl-	[C ₁₈ H ₁₆] [232]	81605-47-2 400–402, 421, 422
382	15 <i>H</i> -Cyclopenta[<i>a</i>]phenanthrene	[C ₁₇ H ₁₂] [216]	219-07-8 97, 323, 520
			
383	15 <i>H</i> -Cyclopenta[<i>a</i>]phenanthrene, 16,17-dihydro-	[C ₁₇ H ₁₄] [218]	482-66-6 81, 278, 323, 338, 400, 425, 520
384	17 <i>H</i> -Cyclopenta[<i>a</i>]phenanthrene	[C ₁₇ H ₁₂] [216]	219-08-9 167
			
385	17 <i>H</i> -Cyclopenta[<i>a</i>]phenanthrene, ethyl-	[C ₁₉ H ₁₆] [244]	71277-92-4 167
386	17 <i>H</i> -Cyclopenta[<i>a</i>]phenanthrene, methyl-	[C ₁₈ H ₁₄] [230]	71277-93-5 167
387	4 <i>H</i> -Cyclopenta[<i>def</i>]phenanthrene	[C ₁₅ H ₁₀] [190]	203-64-5 131, 196, 197, 198, 278, 323, 342, 398, 419
			
388	4 <i>H</i> -Cyclopenta[<i>def</i>]phenanthrene, dimethyl-	[C ₁₇ H ₁₄] [218]	71277-91-3 475
389	4 <i>H</i> -Cyclopenta[<i>def</i>]phenanthrene, ethyl-	[C ₁₇ H ₁₄] [218]	65319-51-9 475
390	4 <i>H</i> -Cyclopenta[<i>def</i>]phenanthrene, methyl-	[C ₁₆ H ₁₂] [204]	58548-39-3 475
391	Cyclopenta[<i>l</i>]phenanthrene, dihydro-	[C ₁₇ H ₁₄] [218]	419
			
392	Fluorantinene, ethylmethyl-	[C ₂₀ H ₁₈] [258]	216
393	Fluoranthene	[C ₁₆ H ₁₀] [202]	206-44-0 1, 4, 5, 8, 11, 13, 20, 21, 29, 30, 43, 44, 51a, 57, 65, 67–69, 72a, 81, 93, 96, 97, 100, 113, 114, 127, 128, 131, 131a, 133a, 137, 138, 150, 155, 157b, 162, 163, 174, 182, 185, 187, 196, 209, 221–223, 230, 231, 239a, 255, 267, 273, 278, 280, 282, 289, 294, 302, 308–311, 314–317, 319, 320, 323, 326, 329–334, 336, 338, 341, 342, 357, 365–368, 370, 372–374, 376, 383, 388, 396, 398, 400, 410, 411, 419, 421–425, 427, 434, 439, 440, 448, 451–457, 459, 467, 477, 479, 484, 490, 491, 494, 496, 500, 502, 503, 519, 520, 524, 530
			
394	Fluoranthene, alkyl-		13, 97, 100, 157b, 162, 163, 182, 273, 317, 323, 329, 332, 342, 459, 479, 484, 490, 491, 496, 500
395	Fluoranthene, dihydro-	[C ₁₆ H ₁₂] [204]	41593-24-2 142
396	Fluoranthene, dihydromethyl-	[C ₁₉ H ₁₄] [218]	71278-25-6 142

Table 6 (cont.)

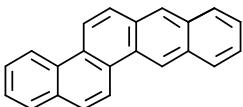
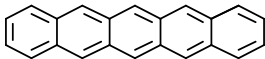
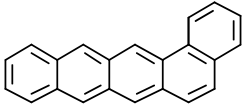
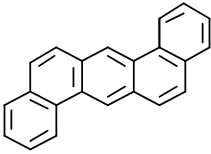
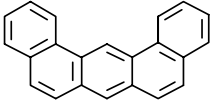
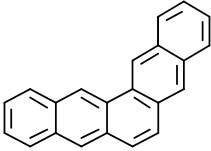
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>TETRACYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
397–399 ^b	Fluoranthene, dimethyl-	[C ₁₈ H ₁₄] [230] 60826-74-6	278, 298, 323, 365, 368, 398, 400–402, 419-422, 459
400	Fluoranthene, 8,9-dimethyl-	[C ₁₈ H ₁₄] [230] 25889-63-8	278, 323, 338, 425, 459
401	Fluoranthene, ethyl-	[C ₁₈ H ₁₄] [230] 55220-72-9	263
402	Fluoranthene, ethylmethyl-	[C ₁₉ H ₁₆] [244] 71277-96-8	416, 420
403	Fluoranthene, hexamethyl-	[C ₂₂ H ₂₂] [286] 71277-97-9	416, 420
A ^m	Fluoranthene, methyl-	[C ₁₇ H ₁₂] [216] 30997-39-8	334, 368, 398, 451-453
404	Fluoranthene, 1-methyl-	[C ₁₇ H ₁₂] [216] 25889-60-5	263, 400-402, 419, 421, 422
405	Fluoranthene, 2-methyl-	[C ₁₇ H ₁₂] [216] 33543-31-6	174, 263, 400-402, 419, 421, 422, 448, 451–453, 530
406	Fluoranthene, 3-methyl-	[C ₁₇ H ₁₂] [216] 1706-01-0	174, 263, 448, 451-453, 530
407	Fluoranthene, 7-methyl-	[C ₁₇ H ₁₂] [216] 23339-05-1	263, 530
408	Fluoranthene, 8-methyl-	[C ₁₇ H ₁₂] [216] 20485-57-8	97, 278, 323, 338, 400–402, 419-422, 425, 454, 455, 459, 530
409–410 ^b	Fluoranthene, pentamethyl-	[C ₂₁ H ₂₀] [272] 71277-98-0	416, 420
411	Fluoranthene, propyl-	[C ₁₉ H ₁₆] [244] 55220-69-4	216
412	Fluoranthene, tetramethyl-	[C ₂₀ H ₁₈] [258] 71277-99-1	416, 420
413	Fluoranthene, trimethyl-	[C ₁₉ H ₁₆] [244] 41637-87-0	400–402, 416, 420–422
<i>PENTACYCLIC: Benzenoid structures</i>			
414	Benzo[<i>b</i>]chrysene	[C ₂₂ H ₁₄] [278] 214-17-5	13, 150, 231, 278, 283, 338, 530
			
415	Pentacene	[C ₂₂ H ₁₄] [278] 135-48-8	150, 198, 231, 283, 342, 529, 530
			
416	Benzo[<i>a</i>]naphthacene	[C ₂₂ H ₁₄] [278] 226-88-0	97, 150, 231, 278, 283, 323, 338, 365, 425, 477, 519, 530
			
417	Dibenzanthracene	[C ₂₂ H ₁₄] [278] 67775-07-9	475
418	Dibenz[<i>a,h</i>]anthracene	[C ₂₂ H ₁₄] [278] 53-70-3	13, 20, 29, 30, 58, 71, 72a, 96, 97, 102, 103, 105a, 106, 122, 131, 131a, 133a, 137, 138, 145, 150, 152–157, 160, 162, 163, 165, 167, 174, 185, 186, 196, 204, 231, 268, 278, 280, 282, 283, 302, 303, 317, 319, 320, 322–324, 326, 329, 332, 334, 336, 338, 341, 342, 356, 365, 410, 414, 417, 419, 423–426, 432, 439, 445, 446, 448, 451–453, 458, 459, 467, 471, 483, 484, 490, 491, 494, 496, 498, 500, 502, 503, 509, 520, 529, 530
			
419	Dibenz[<i>a,j</i>]anthracene	[C ₂₂ H ₁₄] [278] 224-41-9	71, 131, 133a, 150, 174, 231, 283, 320, 357, 336, 419, 423, 424, 529, 530
			
420	Pentaphene	[C ₂₂ H ₁₄] [278] 222-93-5	71, 97, 278, 283, 323, 483, 519
			

Table 6 (cont.)

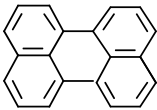
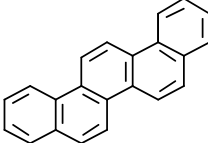
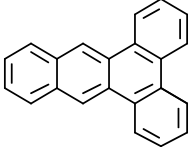
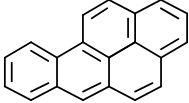
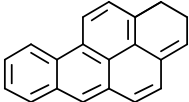
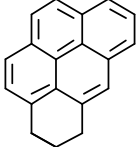
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>PENTACYCLIC: Benzenoid structures (cont.)</i>			
421	Perylene 	[C ₂₀ H ₁₂] [252]	198-55-0 5, 8, 13, 37, 64, 72a, 81, 96, 97, 113, 114, 127, 131, 131a, 133a, 138, 150, 162, 163, 174, 187, 198, 229–231, 239a, 278, 280, 282, 283, 302, 310, 315, 317, 319, 320, 323, 329, 334, 338, 342, 365, 398, 400–402, 419, 421–424, 434, 439, 459, 467, 474, 477, 479, 484, 490, 491, 496, 519, 520, 530
422	Perylene, alkyl-		479
423	Perylene, dimethyl-	[C ₂₂ H ₁₆] [280]	64760-19-6 419
424–425 ^b	Perylene, methyl-	[C ₂₁ H ₁₄] [266]	64031-91-0 419
426	Perylene, 3-methyl-	[C ₂₁ H ₁₄] [266]	24471-47-4 278
427	Picene 	[C ₂₂ H ₁₄] [278]	213-46-7 13, 198, 283, 341, 342, 419, 423, 424, 530
428	Benzo[<i>b</i>]triphenylene 	[C ₂₂ H ₁₄] [278]	215-58-7 150, 231, 319, 320, 326, 336, 356, 409–412, 419, 423, 424, 448–450, 452, 453, 460, 529, 530
429	Benzo[<i>b</i>]triphenylene, methyl-	[C ₂₃ H ₁₆] [292]	64760-20-9 419
A ⁿ	Benzo[<i>a</i>]pyrene	[C ₂₀ H ₁₂] [252]	73467-76-2 324, 529
430	Benzo[<i>a</i>]pyrene 	[C ₂₀ H ₁₂] [252]	50-32-8 1–6, 8, 11–13, 16–20, 20a, 23–25, 27–35, 38, 40–49, 49a, 50, 51, 51a, 52–55, 57, 59–61, 64, 66, 68–70, 72a, 73–76, 78, 80, 81, 83–87, 89–93, 96, 97, 100, 104–108, 110, 112–119, 122, 123, 125–131, 131a, 132, 133, 133a, 135a, 136–139, 141, 143, 145, 146, 148–150, 152–158, 160–165, 167, 169–172, 174, 179, 180a, 181, 184, 185, 187–193, 196–199, 203, 208–210, 214, 215, 217–227, 230, 231, 234, 234a, 236, 238, 239a, 241–246, 248, 249, 251–254, 258, 259, 262, 263, 265a, 265b, 266, 266a, 268, 269, 271–280, 282–284, 286–293, 295–297, 299–303, 305–311, 313–321, 323, 325–327, 329–334, 336–350, 356–359, 363–366, 368–370, 372–374, 376–378, 380, 383–386, 388, 392, 394, 395, 395a, 396–403, 405, 406, 410, 411, 414, 417–419, 421–425, 428–456, 459–461, 466–474, 475a, 476–486, 490, 492–496, 498–507, 511, 512, 514, 515, 515a, 516–521, 523, 524, 526–530
431	Benzo[<i>a</i>]pyrene, alkyl-		13, 81, 100, 97, 278, 317, 323, 327, 329, 332, 342, 434, 479, 496, 520
432	Benzo[<i>a</i>]pyrene, 3,4-dihydro-	[C ₂₀ H ₁₄] [254]	97, 278, 365, 425
433	Benzo[<i>a</i>]pyrene, 7,8-dihydro- 	[C ₂₀ H ₁₄] [254]	17573-23-8 1, 234a, 278, 323, 338
434–435 ^b	Benzo[<i>a</i>]pyrene, dimethyl-	[C ₂₂ H ₁₆] [280]	25167-90-2 59, 234a, 323, 400, 419, 421, 422, 530
436	Benzo[<i>a</i>]pyrene, ethyl-	[C ₂₂ H ₁₆] [280]	71607-83-5 475
437–438 ^b	Benzo[<i>a</i>]pyrene, methyl-	[C ₂₁ H ₁₄] [266]	25167-89-9 234a, 278, 317, 323, 326, 329, 332, 334, 338, 377, 378, 398, 400–402, 419, 421, 422, 425, 459, 500, 509, 530
439	3 <i>H</i> -Benzo[<i>cd</i>]pyrene, 4,5-dihydro- 	[C ₁₉ H ₁₄] [242]	7130-15-6 234a, 400, 419, 421, 422

Table 6 (cont.)

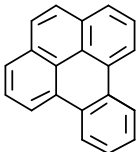
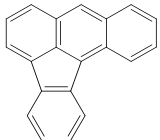
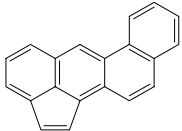
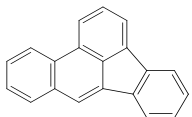
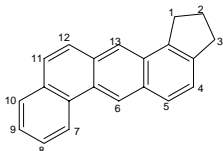
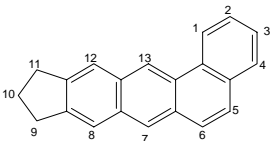
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
440	Benzo[<i>e</i>]pyrene 	[C ₂₀ H ₁₂] [252]	192-97-2 1, 5, 8, 13, 29, 30, 37, 51a, 64, 89, 93, 96, 97, 100, 131, 133, 133a, 137–139, 141, 150, 161, 162, 174, 185, 187, 209, 219, 227, 231, 234a, 239a, 262, 271, 273, 278, 280, 282, 283, 286, 302, 317, 319, 320, 323, 326, 329, 332, 334, 336, 338, 342, 356, 365, 368, 377, 378, 388, 394, 396, 398, 400–402, 410, 411, 417, 419, 421–425, 439, 440, 448–455, 459, 460, 467, 484, 490, 491, 496, 498, 500, 502, 503, 509, 520, 529, 530
441-442 ^b	Benzo[<i>e</i>]pyrene, dimethyl-	[C ₂₂ H ₁₆] [280]	41699-06-3 234a, 400, 419, 421, 422
443-444 ^b	Benzo[<i>e</i>]pyrene, methyl-	[C ₂₁ H ₁₄] [266]	41699-04-1 234a, 377, 378, 398, 400-402, 419, 421, 422, 530
445	Benzo[<i>e</i>]pyrene, trimethyl-	[C ₂₃ H ₁₈] [294]	64760-21-0 174, 234a, 419, 448, 451-453
<i>PENTACYCLIC: Cyclopentanoid-benzenoid structures</i>			
446	Benz[<i>a</i>]aceanthrylene 	[C ₂₀ H ₁₂] [252]	203-33-8 150, 231, 398, 400–402, 419, 421, 422
447	Benz[<i>j</i>]aceanthrylene 	[C ₂₀ H ₁₂] [252]	202-33-5 475, 530
448	Benz[<i>j</i>]aceanthrylene, 1,2-dihydro-	[C ₂₀ H ₁₄] [254]	479-23-2 198, 317, 320, 323, 329, 332, 334, 338, 342, 529, 530
449	Benz[<i>j</i>]aceanthrylene, 1,2-dihydro-3-methyl-	[C ₂₁ H ₁₆] [268]	56-49-5 30, 72a, 196, 204, 278; 283, 320, 323, 338, 356, 410, 423, 424, 426, 510, 529, 530
450	Benz[<i>e</i>]acephenanthrylene 	[C ₂₀ H ₁₂] [252]	205-99-2 5, 11, 13, 20, 29, 97, 106, 107, 122, 127, 128, 131, 131a, 133a, 137, 138, 150, 152–157, 160–163, 165, 167, 174, 185, 187, 229, 231, 267, 268, 278, 302, 319-321, 323, 326, 332, 334, 336, 338, 342, 357, 368, 398, 400–402, 414, 414a, 419, 421–425, 448–453, 461, 467, 474, 484, 490, 491, 496, 497, 500, 502, 503, 509, 518, 519, 529, 530
451	Benz[<i>e</i>]acephenanthrylene, methyl-	[C ₂₁ H ₁₆] [266]	41637-94-9 400–402, 419, 421, 422, 530
452	Benz[<i>e</i>]acephenanthrylene, 10-methyl-	[C ₂₁ H ₁₆] [266]	149021-93-2 475
453	1 <i>H</i> -Benzo[<i>a</i>]cyclopent[<i>h</i>]anthracene, 2,3-dihydro-	[C ₂₁ H ₁₆] [268]	7099-43-6 31–35, 37, 71, 97, 230, 249, 250, 278, 286, 317, 323, 329, 334, 338, 341, 365
			
454	9 <i>H</i> -Benzo[<i>a</i>]cyclopent[<i>j</i>]anthracene, 10,11-dihydro-	[C ₂₁ H ₁₆] [268]	7099-42-5 1, 31–35, 71, 97, 230, 233, 249, 250, 278, 286, 317, 323, 329, 334, 335, 338, 365, 425, 530
			

Table 6 (cont.)

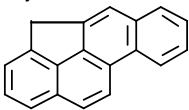
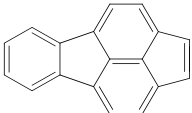
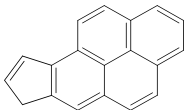
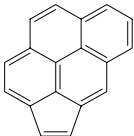
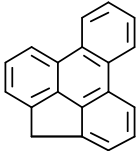
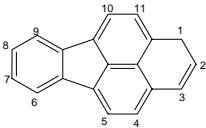
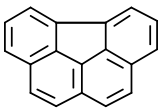
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>PENTACYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
455	4 <i>H</i> -Cyclopenta[<i>def</i>]chrysene 	[C ₁₉ H ₁₂] [240]	202-98-2 419, 530
456	Cyclopenta[<i>cd</i>]fluoranthene 	[C ₁₈ H ₁₀] [226]	193-54-4 475
457	1 <i>H</i> -Cyclopenta[<i>a</i>]pyrene 	[C ₁₉ H ₁₂] [240]	42315-22-0 400–402, 419
458	Cyclopenta[<i>a</i>]pyrene, 3,4-dihydro-	[C ₁₉ H ₁₄] [242]	368, 400–402, 419, 421, 422
459	Cyclopenta[<i>a</i>]pyrene, 3,4-dihydromethyl-	[C ₂₀ H ₁₆] [256]	
460	Cyclopenta[<i>cd</i>]pyrene 	[C ₁₈ H ₁₀] [226]	27208-37-3 131a, 133a, 234a, 419
461	Cyclopenta[<i>cd</i>]pyrene, 3,4-dihydro-	[C ₁₈ H ₁₂] [228]	25732-74-5 475
462	Cyclopenta[<i>cd</i>]pyrene, 3,4-dihydromethyl-	[C ₁₉ H ₁₄] [242]	64760-18-5 475
463	4 <i>H</i> -Cyclopenta[<i>def</i>]triphenylene 	[C ₁₉ H ₁₂] [240]	23992-32-7 419
464	Benzo[<i>fluoranthene</i>	[C ₁₈ H ₁₀] [226]	56832-73-6 5, 216, 417
465	Benzo[<i>fluoranthene</i> , dimethyl-	[C ₂₀ H ₁₄] [254]	416, 420
466	Benzo[<i>fluoranthene</i> , ethyl-	[C ₂₀ H ₁₄] [254]	216
467	Benzo[<i>fluoranthene</i> , methyl-	[C ₁₉ H ₁₂] [240]	416, 420
468	11 <i>H</i> -Benzo[<i>cd</i>]fluoranthene 	[C ₁₉ H ₁₂] [240]	16135-81-2 26, 182, 278, 323, 357, 365, 484, 518
469	Benzo[<i>ghi</i>]fluoranthene 	[C ₁₈ H ₁₀] [226]	203-12-3 50, 51a, 97, 133a, 138, 162, 163, 227, 278, 317, 323, 329, 332, 334, 338, 342, 357, 365, 368, 398, 400–402, 419, 421–425, 454, 455, 459, 461, 467, 474, 484, 490, 491, 496, 497, 500, 510, 520, 530
470	Benzo[<i>ghi</i>]fluoranthene, dimethyl-	[C ₂₀ H ₁₄] [254]	64760-14-1 216, 419
471	Benzo[<i>ghi</i>]fluoranthene, ethyl-	[C ₂₀ H ₁₄] [254]	71265-35-5 475
A °	Benzo[<i>ghi</i>]fluoranthene, methyl-	[C ₁₉ H ₁₂] [240]	51001-44-6 397, 401, 402, 419, 421, 422
472	Benzo[<i>ghi</i>]fluoranthene, 1-methyl-	[C ₁₉ H ₁₂] [240]	71265-21-9 216
473	Benzo[<i>ghi</i>]fluoranthene, 2-methyl-	[C ₁₉ H ₁₂] [240]	71265-22-0 216, 530
474	Benzo[<i>ghi</i>]fluoranthene, 3-methyl-	[C ₁₉ H ₁₂] [240]	71265-23-1 216, 530

Table 6 (cont.)

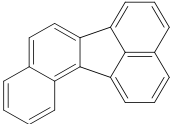
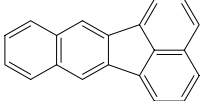
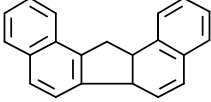
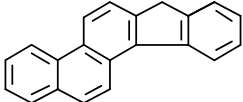
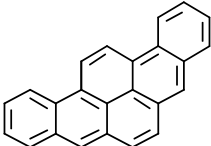
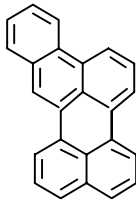
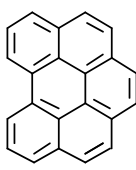
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>PENTACYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
475	Benzo[<i>ghi</i>]fluoranthene, 4-methyl-	[C ₁₉ H ₁₂] [240]	71265-24-2 475
476	Benzo[<i>j</i>]fluoranthene	[C ₂₀ H ₁₂] [252]	205-82-3 11, 13, 20, 97, 106, 131, 131a, 133a, 152–157, 160, 162, 163, 165, 167, 174, 278, 317, 319, 320, 323, 326, 329, 334, 336, 338, 342, 357, 365, 368, 414, 414a, 419, 421–423, 425, 445, 446, 448, 451–453, 459, 467, 474, 484, 490, 491, 496, 497, 500, 502, 503, 509, 529, 530
			
477	Benzo[<i>j</i>]fluoranthene, methyl-	[C ₂₁ H ₁₄] [266]	60826-67-7 419, 421, 422
478	Benzo[<i>k</i>]fluoranthene	[C ₂₀ H ₁₂] [252]	207-08-9 4, 13, 20, 29, 37, 51a, 57, 97, 106, 122, 127, 128, 131, 131a, 133a, 137, 150, 152–157, 160, 162, 163, 167, 174, 185, 187, 228, 230, 231, 268, 278, 317, 319, 320, 323, 326, 329, 332, 334, 336, 338, 342, 357, 365, 368, 388, 398, 400–402, 414, 414a, 419, 421–425, 454, 455, 459, 467, 474, 484, 490, 491, 496, 497, 500, 510, 530
			
479	Benzo[<i>k</i>]fluoranthene, methyl-	[C ₂₁ H ₁₄] [266]	41637-93-8 421, 422, 530
480	13 <i>H</i> -Dibenzo[<i>a, i</i>]fluorene	[C ₂₁ H ₁₄] [266]	239-60-1 37, 89, 97, 227, 230, 278, 286, 323, 336, 338, 342, 425, 530
			
481	11 <i>H</i> -Indeno[2,1- <i>a</i>]phenanthrene	[C ₂₁ H ₁₄] [266]	220-97-3 34, 97, 278, 323, 338, 342, 351, 353, 425
			
<i>HEXACYCLIC: Benzenoid structures</i>			
482	Benzo[<i>rsf</i>]pentaphene	[C ₂₄ H ₁₄] [302]	189-55-9 13, 20, 31, 32, 33–35, 62, 63, 97, 106, 112, 145, 150, 152, 153, 155, 160, 165, 174, 231, 247–250, 268, 283, 286, 317, 319, 320, 322, 323, 326, 329, 332, 334, 336, 338, 342, 356, 358, 365, 389, 414, 414a, 419, 423–425, 445, 446, 448, 451–453, 483, 500, 509, 520, 529, 530
			
483	Benzoperylene	[C ₂₄ H ₁₄] [302]	11057-45-7 283, 475
484	Benzo[<i>b</i>]perylene	[C ₂₄ H ₁₄] [302]	197-70-6 419
			
485	Benzo[<i>ghi</i>]perylene	[C ₂₂ H ₁₂] [276]	191-24-2 1, 8, 13, 29, 37, 57, 68, 69, 89, 93, 96, 97, 127, 131, 131a, 133a, 138, 137, 150, 162, 174, 185, 221, 227, 230, 231, 239a, 273, 278, 280, 286, 302, 308–310, 315, 319, 320, 323, 329–331, 332, 334, 336, 338, 342, 357, 365, 398, 419, 423–425, 448, 451–453, 455, 459, 462, 467, 483, 484, 490–492, 496, 500, 510, 520, 529, 530
			
486-488 ^b	Benzo[<i>ghi</i>]perylene, dimethyl-	[C ₂₄ H ₁₆] [304]	64760-22-1 419
489-490 ^b	Benzo[<i>ghi</i>]perylene, methyl-	[C ₂₃ H ₁₄] [290]	41699-09-6 8, 400, 419
491-492 ^b	Benzo[<i>ghi</i>]perylene, trimethyl-	[C ₂₅ H ₁₈] [318]	64760-23-2 419

Table 6 (cont.)

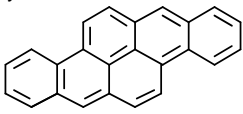
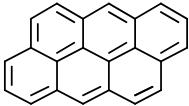
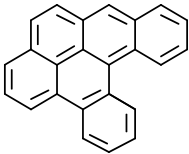
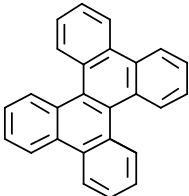
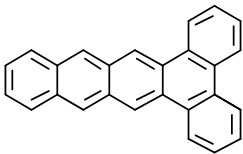
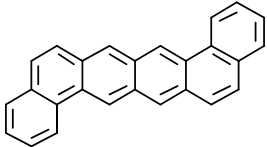
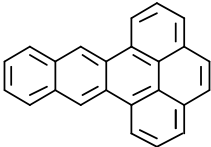
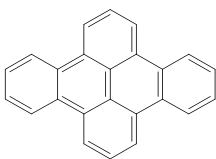

No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>HEXACYCLIC: Benzenoid structures (cont.)</i>			
493	Dibenzo[<i>b,def</i>]chrysene 	[C ₂₄ H ₁₄] [302]	189-64-0 13, 37, 89, 97, 150, 174, 230, 231, 268, 278, 286, 311, 312, 317, 320, 323, 326, 329, 334, 336, 338, 342, 389, 365, 414, 414a, 417, 419, 423–425, 448–453, 477, 483, 500, 509, 519, 520, 529, 530
494	Dibenzo[<i>def,mno</i>]chrysene 	[C ₂₂ H ₁₂] [276]	191-26-4 8, 13, 14, 50, 68, 69, 72a, 96, 97, 113, 114, 131, 133a, 150, 162, 163, 174, 221, 222, 230, 231, 239a, 278, 280, 283, 308, 309, 317, 319, 323, 329, 332, 334, 338, 342, 367, 419, 423–425, 460, 477, 496, 530
495–496 ^b	Dibenzo[<i>def,mno</i>]chrysene, dimethyl-	[C ₂₄ H ₁₆] [304]	64760-24-3 419
497–499 ^b	Dibenzo[<i>def,mno</i>]chrysene, methyl-	[C ₂₃ H ₁₄] [290]	41699-10-9 341, 419
500	Dibenzo[<i>def,mno</i>]chrysene, 6-methyl-	[C ₂₃ H ₁₄] [290]	460
501	Dibenzo[<i>def,p</i>]chrysene 	[C ₂₄ H ₁₄] [302]	191-30-0 35, 97, 100, 106, 145, 150, 152-157, 160, 165, 167, 174, 207, 213, 228, 230, 231, 268, 278, 283, 317, 319, 320, 322, 323, 326, 329, 332, 336, 341, 365, 414, 414a, 419, 423, 424, 445, 446, 498, 500, 503, 509, 518, 519, 520, 529, 530
502	Dibenzo[<i>g,p</i>]chrysene 	[C ₂₆ H ₁₆] [328]	191-68-4 24a
503	Dibenzo[<i>a,c</i>]naphthacene 	[C ₂₆ H ₁₆] [328]	216-00-2 37, 97, 230, 278, 323, 338, 425
504	Dibenzo[<i>a,j</i>]naphthacene 	[C ₂₆ H ₁₆] [328]	227-04-3 97, 278, 323, 338, 425, 435, 477, 483, 490, 491, 519, 520
505	Dibenzo[<i>de,qr</i>]naphthacene 	[C ₂₄ H ₁₄] [302]	193-09-9 150, 205, 231, 278, 317, 323, 329, 332, 338
506	Dibenzo[<i>fg,op</i>]naphthacene 	[C ₂₄ H ₁₄] [302]	192-51-8 150, 231, 234a, 283, 419, 530
507	Dibenzopyrene 	[C ₂₄ H ₁₄] [302]	58615-36-4 35, 234a, 323

Table 6 (cont.)

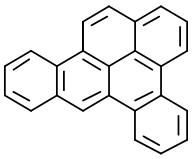
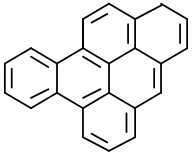
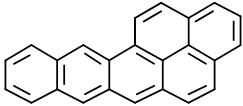
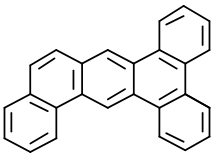
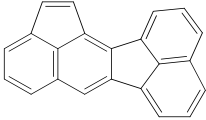
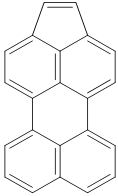
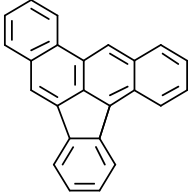
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>HEXACYCLIC: Benzenoid structures (cont.)</i>			
508	Naphtho[1,2,3,4- <i>def</i>]chrysene 	[C ₂₄ H ₁₄] [302]	192-65-4 13, 150, 154, 156, 157, 174, 231, 268, 283, 320, 323, 326, 336, 342, 414, 414a, 419, 423, 424, 529, 530
509	1 <i>H</i> -Naphtho[3,2,1,8- <i>defg</i>]chrysene 	[C ₂₃ H ₁₄] [290]	190-99-8 323, 483
510	Naphtho[2,1,8- <i>gra</i>]naphthacene 	[C ₂₄ H ₁₄] [302]	196-42-9 97, 182, 278, 317, 323, 329, 332, 338, 423, 483, 519, 520, 530
511	Naphtho[1,2- <i>b</i>]triphenylene 	[C ₂₆ H ₁₆] [328]	215-26-9 37, 97, 182, 230, 278, 323, 338, 342, 365, 425, 530
<i>HEXACYCLIC: Cyclopentanoid-benzenoid structures</i>			
512	Acenaphth[1,2- <i>a</i>]acenaphthylene 	[C ₂₂ H ₁₂] [276]	340-99-86 216
513	Acenaphth[1,2- <i>a</i>]acenaphthylene, methyl-	[C ₂₃ H ₁₄] [290]	71265-26-4 216
514	Cyclopenta[<i>cd</i>]perylene 	[C ₂₂ H ₁₂] [276]	189-01-5 216
515	Cyclopenta[<i>cd</i>]perylene, methyl-	[C ₂₃ H ₁₄] [290]	216
516	Dibenz[<i>a,e</i>]aceanthrylene 	[C ₂₄ H ₁₄] [302]	5385-75-1 35, 150, 165, 174, 213, 228, 230, 231, 278, 286, 317, 326, 329, 332, 334, 336, 338, 341, 342, 419, 500, 518, 519, 520, 530

Table 6 (cont.)

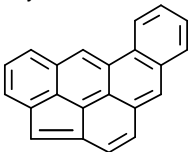
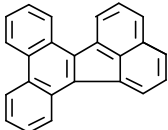
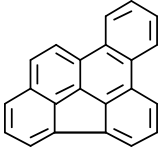
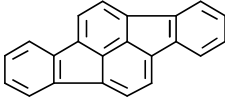
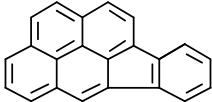
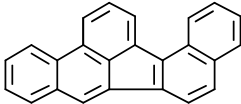
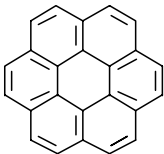
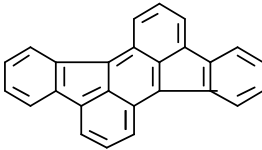
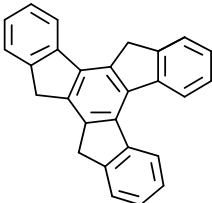
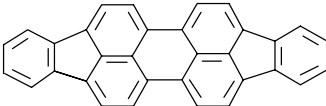
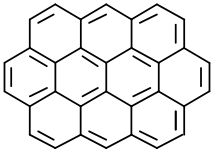
No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>HEXACYCLIC: Cyclopentanoid-benzenoid structures (cont.)</i>			
517	Dibenz[<i>j,mno</i>]aceanthrylene 	[C ₂₂ H ₁₂] [276]	71630-69-8 216
518	Dibenz[<i>j,mno</i>]aceanthrylene, methyl-	[C ₂₃ H ₁₄] [290]	71630-69-8 216
519–520 ^b	Dibenzofluoranthene	60382-88-9	419
521	Dibenzo[<i>j,l</i>]fluoranthene 	[C ₂₄ H ₁₄] [302]	203-18-9 416, 420
522	Indeno[1,2,3,4- <i>defg</i>]chrysene 	[C ₂₂ H ₁₂] [276]	668-30-4 216
523	Indeno[1,2,3,4- <i>defg</i>]chrysene, methyl-	[C ₂₃ H ₁₄] [290]	71277-94-6 216
524	Indeno[1,2,3- <i>cd</i>]fluoranthene 	[C ₂₂ H ₁₂] [276]	193-43-1 11, 13, 93, 97, 106, 133a, 137, 152–157, 160, 163, 165, 167, 174, 268, 323, 326, 414, 419, 425, 448, 451, 452, 496, 500, 509
525	Indeno[1,2,3- <i>cd</i>]fluoranthene, methyl-	[C ₂₃ H ₁₄] [290]	41699-07-4 216
526	Indeno[1,2,3- <i>cd</i>]pyrene 	[C ₂₂ H ₁₂] [276]	193-39-5 8, 11, 13, 20, 29, 97, 106, 131, 131a, 133a, 152–157, 160, 163, 165, 167, 174, 185, 234a, 268, 319, 320, 323, 326, 336, 338, 342, 357, 398, 414, 414a, 419, 421–422, 425, 448, 452, 453, 494, 496, 498, 500, 503, 504, 509, 510, 529, 530
527–528 ^b	Indeno[1,2,3- <i>cd</i>]pyrene, dimethyl-	[C ₂₃ H ₁₄] [290]	64158-99-2 234a, 419
529–530 ^b	Indeno[1,2,3- <i>cd</i>]pyrene, methyl-	[C ₂₃ H ₁₄] [290]	64158-98-1 234a, 419
531	Indeno[1,2,3- <i>cd</i>]pyrene, trimethyl-	[C ₂₅ H ₁₈] [318]	65140-04-7 419
532	Naphth[1,2- <i>e</i>]acephenanthrylene 	[C ₂₄ H ₁₄] [302]	5385-22-8 397, 419
<i>HEPTACYCLIC: Benzenoid structure</i>			
533	Coronene 	[C ₂₄ H ₁₂] [300]	191-07-1 8, 96, 97, 113, 114, 131, 131a, 133a, 137, 138, 150, 174, 188, 189, 198, 222, 231, 278, 280, 319, 320, 323, 327, 329, 332, 334, 338, 342, 365, 398, 419, 423–425, 460, 483, 496, 500, 520, 529, 530
534	Coronene, dimethyl-	[C ₂₆ H ₁₆] [328]	64760-15-2 419
535	Coronene, methyl-	[C ₂₅ H ₁₄] [314]	13119-86-3 419

Table 6 (cont.)

No.	Polycyclic Aromatic Hydrocarbon	CAS RN	References ^a
<i>HEPTACYCLIC: Cyclopentanoid-benzenoid structure</i>			
536	Rubicene 	[C ₂₆ H ₁₄] [326]	197-61-5 177, 323, 351, 353
537	5 <i>H</i> -Tribenzo[<i>a,f,l</i>]trindene, 10,15-dihydro- 	[C ₂₇ H ₁₆] [342]	27096-03-3 323, 351–353, 529 548-35-6
<i>NONACYCLIC: Cyclopentanoid-benzenoid structure</i>			
538	Diindeno[1,2,3- <i>cd</i> :1',2',3'- <i>lm</i>]perylene 	[C ₃₂ H ₁₆] [400]	188-94-3 351–354
<i>DECACYCLIC: Benzenoid structure</i>			
539	Ovalene 	[C ₃₂ H ₁₄] [398]	190-26-1 150, 231, 529, 351–353

^a Many of the citations contain additional references pertinent to the PAH in question.

^b A numerical range indicates that more than one isomer of the PAH was reported.

^c This PAH was not numbered because 1) the positions of the two methyl groups were not specified in the papers cited and 2) PAHs listed as 20 through 29 account for the dimethylnaphthalenes.

^d This PAH was not numbered because 1) the position of the ethyl group was not specified and it could have been either the 1-ethyl- or 2-ethyl-isomer or a mixture of them and 2) PAHs listed as 42 and 43 include both known ethylnaphthalenes.

^e This PAH was not numbered because 1) the position of the methyl group was not specified and it could have been either the 1-methyl- or 2-methyl-isomer or a mixture of them and 2) PAHs listed as 57 and 58 include both known methylnaphthalenes.

^f This PAH was not numbered because 1) the position of the methyl group was not specified in the paper cited and 2) it was uncertain whether two isomers were reported.

^g The positions of the three methyl group were not specified. This isomer was different from five isomers previously reported by Snook *et al.* (421).

^h This PAH was not numbered because 1) the position of the dimethyl groups was not specified in the papers cited and 2) PAHs listed as 179 through 187 account for known dimethylphenanthrenes.

ⁱ This PAH was not numbered because 1) the position of the methyl group was not specified in the papers cited and 2) PAHs listed as 192 through 196 account for the five known methylphenanthrenes.

^j This PAH was not numbered because 1) the position of the methyl group was not specified in the papers cited and 2) PAHs listed as 256 through 260 account for the five known methylfluorenes.

^k This PAH was not numbered because 1) the position of the methyl group was not specified in the papers cited and 2) PAHs listed as 297 through 302 account for the five known methylchrysenes.

^l This PAH was not numbered because 1) the position of the methyl group was not specified in the papers cited and 2) PAHs listed as 328 through 330 account for the three known methylpyrenes.

^m This PAH was not numbered because 1) the position of the methyl group was not specified in the papers cited and 2) PAHs listed as 404 through 408 account for the five known methylfluoranthenes.

ⁿ This PAH was not numbered because in the papers cited, it was unclear whether it was PAH 430 (B[a]P) or PAH 440 (B[e]P) or a mixture thereof.

^o This PAH was not numbered because 1) the position of the methyl group was not specified in the papers cited and 2) PAHs listed as 472 through 475 account for the four known methylbenz[*ghi*]fluoranthenes.

Table 7 summarizes the PAHs identified in CSC that were included in earlier descriptions of proposed structure-tumorigenicity theories.

Examination of Table 7 indicates that most of the PAHs considered in the various theoretical systems designed to establish a relationship between molecular structure and tumorigenicity are totally benzenoid. Only a few PAHs

with a combined benzenoid-cyclopentanoid structure were included in the early studies. LACASSAGNE *et al.* (204) in their discourse on structure-tumorigenicity relationship mentioned a few benzenoid PAHs but their major emphasis was on the structure-tumorigenicity relationship of numerous angular benzacridines. While the number of aza-arenes, including the benzacridines, in CSC is less than the number

Table 7. Tobacco smoke PAHs discussed in various publications on the relationship between PAH structure and tumorigenicity

PAH Discussed	No. in Table 6	Coulson (71)	Fieser et al. (102, 103)	Herndon (150, 231)	Lacassagne et al. (204)	Martin et al. (234a)	Pullman-Pullman (283)	Rubin (356)	Trosko-Upham (440)	Zhang et al. (529)	Y. Zhang (530)
<i>BICYCLIC: Benzeneoid structure</i>											
Naphthalene	1 ^a	X	X	X	X	X	X	-	-	-	X
Naphthalene, dihydro-	4	-	-	-	-	X	-	-	-	-	-
Naphthalene, dihydromethyl-	5-7	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2-dihydro-3-methyl-	15	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	18	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	19	-	-	-	-	X	-	-	-	-	-
Naphthalene, dimethyl-	A ^b	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2-dimethyl-	20	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,3-dimethyl-	21	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,4-dimethyl-	22	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,5-dimethyl-	23	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,6-dimethyl-	24	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,7-dimethyl-	25	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,8-dimethyl-	26	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2,3-dimethyl-	27	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2,6-dimethyl-	28	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2,7-dimethyl-	29	-	-	-	-	X	-	-	-	-	-
Naphthalene, dimethyl-2-ethenyl-	30	-	-	-	-	X	-	-	-	-	-
Naphthalene, dimethylethyl-	31	-	-	-	-	X	-	-	-	-	-
Naphthalene, dimethyl-2-phenyl-	35	-	-	-	-	X	-	-	-	-	-
Naphthalene, dimethyl-1,2,3,4-tetrahydro-	37	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-ethenyl-	38	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-ethenyl-	39	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-ethenylmethyl-	40-41	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-ethyl-	43	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-ethyl-	44	-	-	-	-	X	-	-	-	-	-
Naphthalene, ethylmethyl-	45	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-ethyl-3-methyl-	46	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-ethyl-7-methyl-	49	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-ethyl-8-methyl-	50	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-ethyl-3-methyl-	51	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-ethyl-6-methyl-	54	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-ethyl-7-methyl-	55	-	-	-	-	X	-	-	-	-	-
Naphthalene, hexamethyl-	56	-	-	-	-	X	-	-	-	-	-
Naphthalene, methyl-	A ^c	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-methyl-	57	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-methyl-	58	-	-	-	-	X	-	-	-	-	-
Naphthalene, (1-methylethyl)-	59	-	-	-	-	X	-	-	-	-	-
Naphthalene, methylphenyl-	60	-	-	-	-	X	-	-	-	-	-

Table 7 (cont.)

PAH Discussed	No. in Table 6	Coulson (71)	Fieser et al. (102, 103)	Herndon (150, 231)	Lacassagne et al. (204)	Martin et al. (234a)	Pulliman-Pulliman (283)	Rubin (356)	Trosko-Upham (440)	Zhang et al. (529)	Y. Zhang (530)
BICYCLIC: Benzenoid structure (cont.)											
Naphthalene, methyl-2-phenyl-	61	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-(1-methylpropyl)-	63	-	-	-	-	X	-	-	-	-	-
Naphthalene, methyl-1,2,3,4-tetrahydro-	68	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-methyl-1,2,3,4-tetrahydro-	70	-	-	-	-	X	-	-	-	-	-
Naphthalene, pentamethyl-	73	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-phenyl-	74	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-phenyl-	75	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1-propyl-	77	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2-propyl-	78	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	84	-	-	-	-	X	-	-	-	-	-
Naphthalene, tetramethyl-	85-87	-	-	-	-	X	-	-	-	-	-
Naphthalene, trimethyl-	93	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2,4-trimethyl-	94	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,2,6-trimethyl-	96	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,3,6-trimethyl-	98	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,4,5-trimethyl-	99	-	-	-	-	X	-	-	-	-	-
Naphthalene, 1,6,7-trimethyl-	101	-	-	-	-	X	-	-	-	-	-
Naphthalene, 2,3,6-trimethyl-	102	-	-	-	-	X	-	-	-	-	-
1,1'-Binaphthalene	103	-	-	-	-	X	-	-	-	-	-
1,1'-Binaphthalene, methyl-	106	-	-	-	-	X	-	-	-	-	-
BICYCLIC: Cyclopentanoid-benzenoid structures											
Azulene	156	-	-	X	-	-	X	-	-	-	-
TRICYCLIC: Benzenoid structures											
Anthracene	157	X	X	X	-	-	X	-	X	X	X
Anthracene, dimethyl-	160-162	-	-	-	-	-	X[1]	-	-	-	X[5]
Anthracene, 9,10-dimethyl-	163	-	-	-	-	-	-	-	X	X	X
Anthracene, 1-methyl-	167	-	-	-	-	-	-	-	X	-	-
Anthracene, 2-methyl-	168	-	-	-	-	-	-	-	X	-	-
Anthracene, 9-methyl-	169	-	-	-	-	-	-	-	-	-	X
Anthracene, trimethyl-	171-172	-	-	-	-	-	-	-	-	-	X[1]
Phenanthrene	173	X	X	X	X	-	X	-	X	X	X
Phenanthrene, dimethyl-	178-187	-	-	-	-	-	-	-	-	X[1]	-
Phenanthrene, methyl-	192-196	-	-	-	-	-	-	-	X	-	-
Phenanthrene, tetramethyl-	200-204	-	-	-	-	-	-	-	-	X[1]	-
TRICYCLIC: Cyclopentanoid-benzenoid structures											
Acenaphthylene	208	-	-	X	-	-	-	-	-	-	X
Acenaphthylene, 1,2-dihydro-	209	-	-	-	-	-	-	-	-	-	X
9H-Fluorene	239	-	-	-	-	-	-	-	-	-	X

Table 7 (cont.)

PAH Discussed	No. in Table 6	Coulson (71)	Fieser <i>et al.</i> (102, 103)	Herndon (150, 231)	Lacassagne <i>et al.</i> (204)	Martin <i>et al.</i> (234a)	Pullman (283)	Rubin (356)	Trosko-Upham (440)	Zhang <i>et al.</i> (529)	Y. Zhang (530)
TETRACYCLIC: Benzenoid structures											
Naphthacene	264	X	-	-	-	-	X	-	-	-	X
Benz[<i>a</i>]anthracene	266	X	X	-	X	-	X	-	-	-	X
Benz[<i>a</i>]anthracene, dimethyl-	268-269	X[8] ^d	-	-	-	-	-	-	-	X[6]	X[23]
Benz[<i>a</i>]anthracene, 7,12-dimethyl-	270	X	-	-	X	-	X	X	X	X	X
Benz[<i>a</i>]anthracene, ethyl-	271	-	-	-	-	-	-	-	-	X[1]	-
Benz[<i>a</i>]anthracene, 1-methyl-	274	X	-	-	-	-	-	-	-	-	X
Benz[<i>a</i>]anthracene, 2-methyl-	275	X	-	-	-	-	-	-	-	-	X
Benz[<i>a</i>]anthracene, 3-methyl-	276	X	-	-	-	-	-	-	-	-	X
Benz[<i>a</i>]anthracene, 4-methyl-	277	X	-	-	-	-	-	-	-	-	X
Benz[<i>a</i>]anthracene, 5-methyl-	278	X	-	-	-	-	-	-	-	X	X
Benz[<i>a</i>]anthracene, 6-methyl-	279	X	-	-	-	-	-	-	-	X	-
Benz[<i>a</i>]anthracene, 8-methyl-	280	X	-	-	-	-	-	-	-	X	X
Benz[<i>a</i>]anthracene, 9-methyl-	281	X	-	-	X	-	-	-	-	X	X
Benz[<i>a</i>]anthracene, 10-methyl	282	X	-	-	-	-	-	-	-	X	X
Benz[<i>a</i>]anthracene, 12-methyl-	283	X	-	-	-	-	-	-	-	X	X
Benz[<i>a</i>]anthracene, propyl-	285	-	-	-	-	-	-	-	-	X[1]	-
Benz[<i>a</i>]anthracene, tetramethyl-	286	X[1]	-	-	-	-	-	-	-	X[2]	-
Benz[<i>a</i>]anthracene, trimethyl-	287-288	X[3]	-	-	-	-	-	-	-	X[3]	X[13]
Benzo[<i>c</i>]phenanthrene	290	X	-	X	-	-	X	-	-	-	X
Benzo[<i>c</i>]phenanthrene, methyl	291	X[4]	-	X	-	-	X	-	X	X[6]	X[6]
Chrysene	292	X	-	-	X	-	-	-	X	X	X[10]
Chrysene, dimethyl-	294	-	-	-	-	-	-	-	-	-	X
Chrysene, 1-methyl-	297	-	-	-	-	-	-	-	-	X	X
Chrysene, 2-methyl-	298	-	-	-	-	-	-	-	-	X	X
Chrysene, 3-methyl-	299	-	-	-	-	-	-	-	-	X	X
Chrysene, 4-methyl-	300	-	-	-	-	-	-	-	-	X	X
Chrysene, 5-methyl-	301	-	-	-	-	-	-	-	-	X	X
Chrysene, 6-methyl-	302	-	-	-	-	-	-	-	-	X	X
Triphenylene	307	X	-	X	-	-	X	-	X	X	X
Triphenylene, methyl-	309	-	-	-	-	-	-	-	-	-	X[1]
Pyrene	311	X	-	X	-	X	X	-	X	-	X
Pyrene, dihydro-	315	-	-	-	-	X	-	-	-	-	-
Pyrene, dimethyl-	316-318	-	-	-	-	X	-	-	-	-	-
Pyrene, 3,4-dimethylene-	321	-	-	-	-	X	-	-	-	-	-
Pyrene, hexamethyl-	326	-	-	-	-	X	-	-	-	-	-
Pyrene, 1-hexyl-	327	-	-	-	-	X	-	-	-	-	-
Pyrene, methyl-	A ^c	-	-	-	-	X	-	-	-	-	-
Pyrene, 1-methyl-	328	-	-	-	-	X	-	-	-	-	X
Pyrene, 2-methyl-	329	-	-	-	-	X	-	-	-	-	X
Pyrene, 4-methyl-	330	-	-	-	-	X	-	-	-	-	X

Table 7 (cont.)

PAH Discussed	No. in Table 6	Coulson (71)	Fieser et al. (102, 103)	Herndon (150, 231)	Lacassagne et al. (204)	Martin et al. (234a)	Pullman-Pullman (283)	Rubin (356)	Trosko-Upham (440)	Zhang et al. (529)	Y. Zhang (530)
<i>TETRACYCLIC: Benzenoid structures (cont.)</i>											
Pyrene, pentamethyl-	332-334	-	-	-	-	X	-	-	-	-	-
Pyrene, tetramethyl-	338-341	-	-	-	-	X	-	-	-	-	-
Pyrene, trimethyl-	342-344	-	-	-	-	X	-	-	-	-	-
<i>TETRACYCLIC: Cyclopentanoid-benzenoid structures</i>											
7H-Benzo[<i>c</i>]fluorene	374	-	-	-	-	-	-	-	-	-	X
Fluoranthene	393	-	-	X	-	-	-	-	-	-	X
Fluoranthene, 2-methyl-	405	-	-	-	-	-	-	-	-	-	X
Fluoranthene, 3-methyl-	406	-	-	-	-	-	-	-	-	-	X
Fluoranthene, 7-methyl-	407	-	-	-	-	-	-	-	-	-	X
Fluoranthene, 8-methyl-	408	-	-	-	-	-	-	-	-	-	X
<i>PENTACYCLIC: Benzenoid structures</i>											
Benzol[<i>b</i>]chrysene	414	-	-	X	-	-	X	-	-	-	X
Pentacene	415	-	-	X	-	-	X	-	-	X	X
Benzol[<i>a</i>]naphthacene	416	-	-	X	-	-	X	-	-	-	X
Dibenz[<i>a,h</i>]anthracene	418	X	X	X	X	-	X	X	-	X	X
Dibenz[<i>a,j</i>]anthracene	419	X	-	X	-	-	X	-	-	X	X
Pentaphene	420	X	-	-	-	-	X	-	-	-	X
Perylene	421	-	-	X	-	-	X	-	-	-	X
Picene	427	-	-	-	-	-	X	-	-	-	-
Benzol[<i>b</i>]triphenylene	428	-	-	X	-	-	X	X	-	X	X
Benzopyrene	A ^o	-	-	-	-	-	-	-	-	X	-
Benzol[<i>a</i>]pyrene	430	-	-	X	-	X	X	X	X	X	X
Benzol[<i>a</i>]pyrene, 7,8-dihydro-	433	-	-	-	-	X	-	-	-	-	-
Benzol[<i>a</i>]pyrene, dimethyl-	434-435	-	-	-	-	X	-	-	-	-	X[9]
Benzol[<i>a</i>]pyrene, methyl-	437-438	-	-	-	-	X	-	-	-	-	X[1]
3H-Benzo[<i>c,d</i>]pyrene, 4,5-dihydro-	439	-	-	-	-	X	-	-	-	-	-
Benzol[<i>e</i>]pyrene	440	-	-	X	-	X	X	X	X	X	X
Benzol[<i>e</i>]pyrene, dimethyl-	441-442	-	-	-	-	X	-	-	-	-	-
Benzol[<i>e</i>]pyrene, methyl-	443-444	-	-	-	-	X	-	-	-	-	X[12]
Benzol[<i>e</i>]pyrene, trimethyl-	445	-	-	-	-	X	-	-	-	-	-
<i>PENTACYCLIC: Cyclopentanoid-benzenoid structures</i>											
Benz[<i>a</i>]aceanthrylene	446	-	-	X	-	-	-	-	-	-	X
Benz[<i>j</i>]aceanthrylene, 1,2-dihydro-	448	-	-	-	-	-	-	-	-	X	X
Benz[<i>j</i>]aceanthrylene, 1,2-dihydro-3-methyl-	449	-	-	-	X	-	X	X	-	X	X
Benz[<i>e</i>]acephenanthrylene	450	-	-	X	-	-	-	-	-	X	X
Benz[<i>e</i>]acephenanthrylene, methyl-	451	-	-	-	-	-	-	-	-	-	X[6]
1H-Benzo[<i>a</i>]cyclopent[<i>h</i>]anthracene, 2,3-dihydro-	453	X	-	-	-	-	-	-	-	-	-

Table 7 (cont.)

PAH Discussed	No. in Table 6	Coulson (71)	Fieser <i>et al.</i> (102, 103)	Herndon (150, 231)	Lacassagne <i>et al.</i> (204)	Martin <i>et al.</i> (234a)	Pullman-Pullman (283)	Rubin (356)	Trosko-Upham (440)	Zhang <i>et al.</i> (529)	Y. Zhang (530)
PENTACYCLIC: Cyclopentanoid-benzenoid structures											
9 <i>H</i> -Benzo[a]cyclopent[<i>h</i>]anthracene, 10,11-dihydro-	454	X	-	-	-	-	-	-	-	-	X
4 <i>H</i> -Cyclopenta[<i>def</i>]chrysene	455	-	-	-	-	-	-	-	-	-	X
Cyclopenta[<i>cd</i>]pyrene	460	-	-	-	-	X	-	-	-	-	-
Benzo[<i>ghi</i>]fluoranthene	469	-	-	-	-	-	-	-	-	-	X
Benzo[<i>ghi</i>]fluoranthene, 2-methyl-	473	-	-	-	-	-	-	-	-	-	X
Benzo[<i>ghi</i>]fluoranthene, 3-methyl-	474	-	-	-	-	-	-	-	-	-	X
Benzo[<i>j</i>]fluoranthene	476	-	-	-	-	-	-	-	-	X	X
Benzo[<i>k</i>]fluoranthene	478	-	-	X	-	-	-	-	-	-	X
Benzo[<i>k</i>]fluoranthene, methyl-	479	-	-	-	-	-	-	-	-	-	X[3]
13 <i>H</i> -Dibenzo[<i>a, j</i>]fluorene	480	-	-	-	-	-	-	-	-	-	X
HEXACYCLIC: Benzenoid structures											
Benzo[<i>rs</i>]pentafluorene	482	-	-	X	-	-	-	X	-	X	X
Benzoperylene	483	-	-	-	-	-	-	-	-	-	-
Benzo[<i>ghi</i>]perylene	485	-	-	X	-	-	-	-	-	X	X
Dibenzo[<i>b, def</i>]chrysene	493	-	-	X	-	-	X	-	-	X	X
Dibenzo[<i>def, mno</i>]chrysene	494	-	-	X	-	-	X	-	-	-	X
Dibenzo[<i>def, p</i>]chrysene	501	-	-	X	-	-	X	-	-	X	X
Dibenzo[<i>a, j</i>]naphthacene	504	-	-	-	-	-	X	-	-	-	-
Dibenzo[<i>de, q</i>]naphthacene	505	-	-	X	-	-	-	-	-	-	-
Dibenzo[<i>fg, o</i>]naphthacene	506	-	-	X	-	-	X	-	-	-	X
Dibenzopyrene	507	-	-	-	-	X	-	-	-	-	-
Naphtho[1,2,3,4- <i>def</i>]chrysene	508	-	-	X	-	-	X	-	-	X	X
Naphtho[2,1,8- <i>qra</i>]naphthacene	510	-	-	X	-	-	X	-	-	-	X
Naphtho[1,2- <i>bj</i>]triphenylene	511	-	-	X	-	-	X	-	-	-	X
HEXACYCLIC: Cyclopentanoid-benzenoid structures											
Dibenzo[<i>a, e</i>]aceanthrylene	516	-	-	X	-	-	-	-	-	-	X
Indeno[1,2,3- <i>cd</i>]pyrene	526	-	-	-	-	X	-	-	-	X	X
Indeno[1,2,3- <i>cd</i>]pyrene, dimethyl-	527-528	-	-	-	-	X	-	-	-	-	-
Indeno[1,2,3- <i>cd</i>]pyrene, methyl-	529-530	-	-	-	-	X	-	-	-	-	-
HEPTACYCLIC: Benzenoid structure											
Coronene	533	-	-	X	-	-	-	-	-	X	X
HEPTACYCLIC: Cyclopentanoid-benzenoid structure											
5 <i>H</i> -Tribenzo[<i>a, f, i</i>]trindene, 10,15-dihydro-	537	-	-	-	-	-	-	-	-	X	-
DECACYCLIC: Benzenoid structure											
Ovalene	539	-	-	X	-	-	-	-	-	X	-

^a Number is that used in the cigarette mainstream smoke PAH catalogue in Table 6; the CAS No. is shown in Table 6.

^b The positions of the two methyl groups were not specified.

^c The position of the methyl group was not specified.

^d Number in square brackets indicates the number of isomers included in the study.

^e The nature of the benzopyrene was not specified.

of PAHs, nearly 200 have been identified, many by the USDA group at Athens, GA (418). With the knowledge that CSC contains non-tumorigenic PAHs that have been shown to substantially reduce the tumorigenicity of several potentially tumorigenic PAHs, consideration of the study of LACASSAGNE *et al.* raises several interesting questions with regard to tobacco smoke composition. 1) Do any of the benzacridines or other aza-arenes in CSC partially or totally inhibit the tumorigenicity of the tumorigenic benzacridines or other aza-arenes? 2) Do any of the benzacridines inhibit the tumorigenicity of tumorigenic PAHs? Do any of the PAHs reduce the tumorigenicity of the tumorigenic aza-arenes?

The mixture known as CSC is so complex that it is not possible to ascribe its biological activity to any individual component because of the known behavior of that component when administered individually.

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