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# 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 benzenoider 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 tumorigénicité de nombreux

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PAHs, beaucoup d'études ont été menées en vue d'examiner la relation entre les structures des PAHs et leurs tumorigénicités 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 azaarenes 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 *et al.* | 77 | 339 |
| 1963 | Philip Morris | 61 | 278 |
| 1963 | Rodgman *et al.* | 77 | 340 |
| 1964 | Elmenhorst and Reckzeh | 70 | 97 |
| 1965 | Rodgman *et al*. | 85 | 338 |
| 1967 | Rodgman and Woosley | 85 | 342 |
| 1968 | Stedman | 79 | 425 |
| 1975 | Roberts *et al*. | 206 | 303 |
| 1976 | Snook *et al.* | 252 [b] | 421 |
| 1977 | Snook *et al.* | 157 [b] | 419 |
| 1978 | Snook *et al.* | 438 [b] | 420 |
| 1980 | Ishiguro and Sugawara | 191 | 176 |
| 1997 | Williams *et al*. | 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

[b] Numerous 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.

[c] During 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 |

[d] At 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 B*a*P as such contributes to the carcinogenicity of tobacco smoke condensate, we can certainly agree that the concentration of B*a*P may be regarded as an 'indicator' of carcinogenic PAH in tobacco smoke condensate . . . While B*a*P 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 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

[e]All 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, from 1968 to 1978, no new design technology was generated in the NCI Smoking and Health Program on the "less hazardous" cigarette.

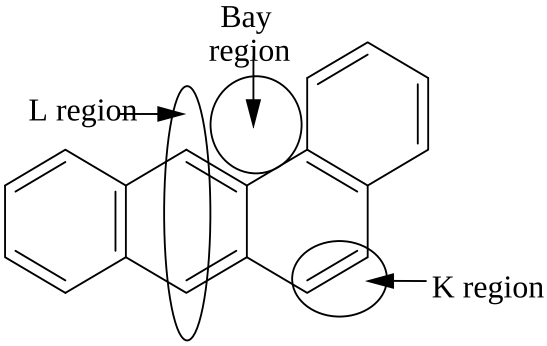


**Figure 1. The L region, K region, and bay region of benz[*a*]anthracene**

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 |
|---|---|---|---|---|
| *Monocyclic* | | | | |
| Benzene [b] | 71-43-2 | — | I | no |
| *Bicyclic* | | | | |
| Naphthalene | 91-20-3 | 1 | II | no |
| *Tricyclic* | | | | |
| Anthracene | 120-12-7 | 157 | III | no |
| Phenanthrene | 85-01-8 | 173 | IV | no |
| *Tetracyclic* | | | | |
| Naphthacene | 92-24-0 | 264 | VII | no |
| Benz[*a*]anthracene | 56-55-3 | 266 | VI | ? |
| Benz[*a*]anthracene, 2,10-dimethyl- | — | — | XLIII | ? |
| Benz[*a*]anthracene, 7,12-dimethyl- | 57-97-6 | 270 | XLII | yes |
| Benz[*a*]anthracene, 7-methyl- | 2541-69-7 | — | XLIV | yes |
| Benzo[*c*]phenanthrene | 195-19-7 | 290 | V | yes |
| Benzo[*c*]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 |
| *Pentacyclic* | | | | |
| Benzo[*b*]chrysene | 214-17-5 | 414 | XXIII | no |
| Benzo[*c*]chrysene | 194-69-4 | — | XIII | yes |
| Benzo[*g*]chrysene | 196-78-1 | — | XIV | yes |
| Pentacene | 135-48-8 | 415 | XVIII | no |
| Benzo[*a*]naphthacene | 226-88-0 | 416 | XVII | no |
| Dibenz[*a,h*]anthracene | 53-70-3 | 418 | XII | yes |
| Dibenz[*a,j*]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[*b*]triphenylene | 215-58-7 | 428 | XX | no |
| Benzo[*a*]pyrene | 50-32-8 | 430 | XI | yes |
| Benzo[*a*]pyrene, 2-methyl- | — | 437–438 [d] | XLVII | yes |
| Benzo[*a*]pyrene, 3-methyl- | — | — | XLVII | yes |
| Benzo[*a*]pyrene, 5-methyl- | — | — | XLVII | yes |
| Benzo[*a*]pyrene, 6-methyl- | 2381-39-7 | — | XLVII | yes |
| Benzo[*a*]pyrene, 7-methyl- | 63041-77-0 | — | XLVII | yes |
| Benzo[*a*]pyrene, 8-methyl- | 63041-76-9 | — | XLVII | no |
| Benzo[*a*]pyrene, 9-methyl- | — | — | XLVII | no |
| Benzo[*e*]pyrene | 192-97-2 | 440 | XVI | no |
| Dibenzo[*b,g*]phenanthrene | 195-06-2 | — | XXIV | no |
| Dibenzo[*c,g*]phenanthrene | 188-52-3 | — | XXII | no |
| Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl- [e] | 56-49-5 | 449 | XLV | yes |
| *Hexacyclic* | | | | |
| Anthra[1,2-*a*]anthracene | 195-00-6 | — | XXXV | no |
| Benzo[*c*]pentaphene | 222-54-8 | — | XXXVII | no |
| Benzo[*rst*]pentaphene | 189-55-9 | 482 | LIV | (yes) [f] |
| Benzo[*pqr*]picene | 189-96-8 | — | LVII | no |
| Dibenzo[*b,def*]chrysene | 189-64-0 | 493 | XXVII | yes |
| Dibenzo[*b,k*]chrysene | 217-54-9 | — | XXXVI | no |
| Dibenzo[*c,mno*]chrysene | 196-28-1 | — | LVI | no |
| Dibenzo[*def,mno*]chrysene | 191-26-4 | 494 | XXXI | no |
| Dibenzo[*def,p*]chrysene | 191-30-0 | 501 | XXVI | yes |
| Dibenzo[*a,j*]naphthacene | 227-04-3 | 504 | XXXIII | no |
| Dibenzo[*a,l*]naphthacene | 226-86-8 | — | XXXIV | no |
| Dibenzo[*fg,op*]naphthacene | 192-51-8 | 506 | XXIX | no |
| Naphtho[1,2,3,4-*def*]chrysene | 192-65-4 | 508 | XXVIII | ? |
| Naphtho[2,1,8-*qra*]naphthacene | 196-42-9 | 510 | XXX | no |
| Naphtho[1,2-*b*]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 |
|---|---|---|---|---|
| *Heptacyclic* | | | | |
| Benzo[*a*]naphtho[8,1,2-*lmn*]naphthacene | 190-01-2 | — | LV | no |
| Dibenzo[*fg,qr*]pentacene | 197-74-0 | — | XL | no |
| *Octacyclic* | | | | |
| Dinaphtho[1,2-*b*:1,2-*k*]chrysene | 214-13-1 | — | XXXIX | no |
| Naphthaceno[2,1,12,11-*opqra*]naphthacene | 188-42-1 | — | LVIII | ? [g] |
| Phenanthro[1,10,9,8-*opqra*]perylene | 190-39-6 | — | XLI | no |
| *Nonacyclic* | | | | |
| Dinaphtho[1,2-*b*:1,2-*n*]perylene | — | — | XXXVIII | no |
| *Decacyclic* | | | | |
| 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[*rst*]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[*a*]anthracene | | | | 219, 227 |
| Benzo[*ghi*]perylene | | | 68 | 69, 221, 227 |
| Benzo[*a*]pyrene | | | 61, 68, 70, 217 | 6, 48, 100, 184, 221, 395, 518 |
| Benzo[*e*]pyrene | | | | 219 |
| Dibenzo[*def,mno*]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 of 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].

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 non-carcinogenic 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.

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[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. 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 potently 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 indenes (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 benzocyclopentanthracenes 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-HOÏ (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-(methylnitrosoamino)-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) [g], 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.

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[g] 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'*-nitrosonornicotine (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**

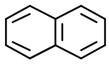
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | | *BICYCLIC: Benzenoid structures* | | |
| 1 | Naphthalene  | [$C_{10}H_8$] [128] | 91-20-3 | 8, 13–15, 20, 29, 30, 32, 33, 50, 57, 65, 71, 72a, 81, 93, 95, 97, 102, 103, 113, 114, 124, 126–128, 135, 137, 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<br>65338-07-0 | 234a, 264 |
| 38 | Naphthalene, 1-ethenyl- | [$C_{12}H_{10}$] [154] | 826-74-4<br>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.*)**

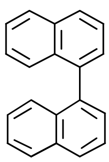
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *BICYCLIC: Benzenoid structures (cont.)* | | | |
| 49 | Naphthalene, 1-ethyl-7-methyl- | $[C_{13}H_{14}]$ [170] | 31032-92-5 | 95, 234a, 265 |
| 50 | Naphthalene, 1-ethyl-8-methyl- | $[C_{13}H_{14}]$ [170] | 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.*)**

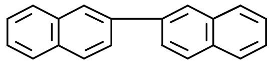
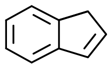
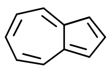
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *BICYCLIC: Benzenoid structures (cont.)* | | | |
| 104 | 1,1'-Binaphthylene, dimethyl- | [$C_{22}H_{18}$] [282] | 71265-39-9 | 216 |
| 105 | 1,1'-Binaphthylene, ethyl- | [$C_{22}H_{18}$] [282] | 71277-81-1 | 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 |
| | *BICYCLIC: Cyclopentanoid-benzenoid structures* | | | |
| 111 | 1*H*-Indene  | [$C_9H_8$] [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*H*-Indene, diethyl- | [$C_{13}H_{16}$] [172] | 71278-05-2 | 416, 420 |
| 113 | 1*H*-Indene, 2,3-dihydro- | [$C_9H_{10}$] [118] | 496-11-7 | 134, 135, 175, 180, 260, 261, 390, 392 |
| 114 | 1*H*-Indene, 2,3-dihydrodimethyl- | [$C_{11}H_{14}$] [146] | 53563-67-0 | 237, 257, 260, 261, 392, 474 |
| 115 | 1*H*-Indene, 2,3-dihydro-1,2-dimethyl- | [$C_{11}H_{14}$] [146] | 17057-82-8 | 263, 264, 392 |
| 116 | 1*H*-Indene, 2,3-dihydroethyl- | [$C_{11}H_{14}$] [146] | 71278-02-9 | 260, 261, 264, 392 |
| 117 | 1*H*-Indene, 2,3-dihydromethyl- | [$C_{10}H_{12}$] [132] | 27133-93-3 | 126, 237, 240, 257, 260, 261, 361 |
| 118 | 1*H*-Indene, 2,3-dihydro-1-methyl- | [$C_{10}H_{12}$] [132] | 767-58-8 | 126, 168, 261 |
| 119 | 1*H*-Indene, 2,3-dihydro-2-methyl- | [$C_{10}H_{12}$] [132] | 824-63-5 | 260, 261 |
| 120 | 1*H*-Indene, 2,3-dihydro-4-methyl- | [$C_{10}H_{12}$] [132] | 824-22-6 | 180 |
| 121 | 1*H*-Indene, 2,3-dihydro-5-methyl- | [$C_{10}H_{12}$] [132] | 874-35-1 | 264, 392 |
| 122 | 1*H*-Indene, 2,3-dihydrotrimethyl- | [$C_{12}H_{16}$] [160] | 36541-18-1 | 257, 264, 392 |
| 123 | 1*H*-Indene, dimethyl- | [$C_{11}H_{12}$] [144] | 29348-63-8 | 8, 237, 257, 392, 400–402, 416, 420–422 |
| 124 | 1*H*-Indene, dimethylethyl- | [$C_{13}H_{16}$] [172] | 71278-06-3 | 8, 416, 420 |
| 125 | 1*H*-Indene, 5,6-dimethyl-2-phenyl- | [$C_{17}H_{16}$] [220] | | 22 |
| 126 | 1*H*-Indene, 2-(3',4'-dimethylphenyl)- | [$C_{17}H_{16}$] [220] | | 22 |
| 127 | 1*H*-Indene, ethyl- | [$C_{11}H_{12}$] [144] | 58924-35-9 | 8, 257, 416, 420 |
| 128 | 1*H*-Indene, ethylmethyl- | [$C_{12}H_{14}$] [158] | 77227-01-1 | 416, 420 |
| 129 | 1*H*-Indene, ethylpentamethyl- | [$C_{16}H_{22}$] [214] | 71278-07-4 | 416, 420 |
| 130 | 1*H*-Indene, heptamethyl- | [$C_{16}H_{22}$] [214] | 77242-77-4 | 416, 420 |
| 131 | 1*H*-Indene, hexamethyl- | [$C_{15}H_{20}$] [200] | 71278-08-5 | 416, 420 |
| 132–134 [b] | 1*H*-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*H*-Indene, 1-methyl- | [$C_{10}H_{10}$] [130] | 767-59-9 | 126, 400–402, 416, 420–422 |
| 136 | 1*H*-Indene, 2-methyl- | [$C_{10}H_{10}$] [130] | 2177-47-1 | 576, 400-402, 416, 420 |
| 137 | 1*H*-Indene, 3-methyl- | [$C_{10}H_{10}$] [130] | 767-60-2 | 263, 392, 400, 416, 420–422 |
| 138 | 1*H*-Indene, 1-methylene- | [$C_{10}H_8$] [128] | 2471-84-3 | 392 |
| 139 | 2*H*-Indene, 2-methylene- | [$C_{10}H_8$] [128] | 6596-86-7 | 392 |
| 140 | 1*H*-Indene, 4-methyl-2-(2'-methylphenyl)- | [$C_{17}H_{16}$] [220] | | 22 |
| 141 | 1*H*-Indene, 5-methyl-2-(4'-methylphenyl)- | [$C_{17}H_{16}$] [220] | | 22 |
| 142 | 1*H*-Indene, 6-methyl-2-(4'-methylphenyl)- | [$C_{17}H_{16}$] [220] | | 22 |
| 143 | 1*H*-Indene, 7-methyl-2-(2'-methylphenyl)- | [$C_{17}H_{16}$] [220] | | 22 |
| 144 | 1*H*-Indene, 7-(4'-methylphenyl)- | [$C_{16}H_{14}$] [206] | | 22 |
| 145 | 1*H*-Indene, pentamethyl- | [$C_{14}H_{18}$] [186] | 71278-09-6 | 416, 420 |
| 146 | 1*H*-Indene, phenyl- | [$C_{15}H_{12}$] [192] | 38638-41-4 | 166, 416, 420 |
| 147 | 1*H*-Indene, 2-phenyl- | [$C_{15}H_{12}$] [192] | 4505-48-0 | 22 |
| 148 | 1*H*-Indene, phenyltrimethyl- | [$C_{18}H_{18}$] [234] | | 22 |
| 149–152 [b] | 1*H*-Indene, tetramethyl- | [$C_{13}H_{16}$] [172] | 27135-78-0 | 8, 257, 416, 420 |
| 153–155 [b] | 1*H*-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.*)**

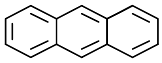
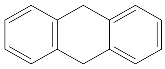
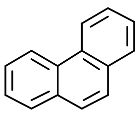
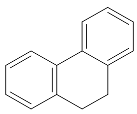
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *TRICYCLIC: Benzenoid structures* | | | |
| 157 | Anthracene  | [$C_{14}H_{10}$] [178] | 120-12-7 | 1, 4, 5, 8, 11, 13, 22, 29, 30, 32–34, 43, 44, 50, 51a, 57, 61, 67-69, 71, 72a, 74, 76, 81, 93, 96, 97, 100, 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, dihydrodimethylene- | [$C_{16}H_{12}$] [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.*)**

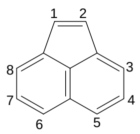
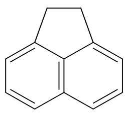
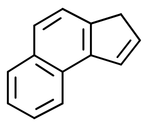
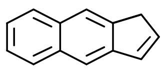
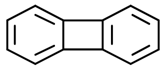
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *TRICYCLIC: Benzenoid structures (cont.)* | | | |
| 190 | Phenanthrene, ethylmethyl- | $[C_{17}H_{16}]$ [220] | 71607-66-4 | 475 |
| 191 | Phenanthrene, hexamethyl- | $[C_{20}H_{22}]$ [262] | 71607-67-5 | 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 |
| | *TRICYCLIC: Cyclopentanoid-benzenoid structures* | | | |
| 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-dihydrodimethyl- | $[C_{14}H_{14}]$ [182] | 60684-29-9 | 400–402, 416, 420–422 |
| 211 | Acenaphthylene, 1,2-dihydromethyl- | $[C_{13}H_{12}]$ [168] | 36541-21-6 | 379, 400–402, 416, 420–422 |
| 212 | Acenaphthylene, 1,2-dihydrotetramethyl- | $[C_{16}H_{18}]$ [210] | 60826-72-4 | 400–402, 416, 420–422 |
| 213–214 [b] | Acenaphthylene, 1,2-dihydrotrimethyl- | $[C_{15}H_{16}]$ [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*H*-Benz[*e*]indene  | $[C_{13}H_{10}]$ [166] | 232-54-2 | 397 |
| 230 | 1*H*-Benz[*e*]indene, dimethyl- | $[C_{15}H_{14}]$ [194] | | 416, 420 |
| 231 | 1*H*-Benz[*e*]indene, methyl- | $[C_{14}H_{12}]$ [180] | 64031-90-9 | 397 |
| 232 | 1*H*-Benz[*f*]indene  | $[C_{13}H_{10}]$ [166] | 268-40-6 | 398, 400–402, 421, 422 |
| 233 | 1*H*-Benz[*f*]indene, dimethyl- | $[C_{15}H_{14}]$ [194] | 60826-71-3 | 400–402, 416, 420–422 |
| 234 | 1*H*-Benz[*f*]indene, ethylmethyl- | $[C_{16}H_{16}]$ [208] | 71265-34-4 | 416, 420 |
| 235–237 [b] | 1*H*-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.*)**

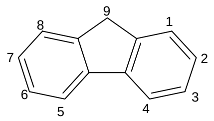
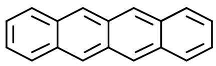
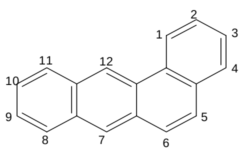
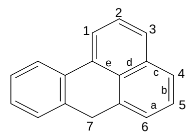
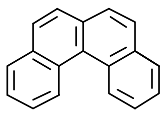
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *TRICYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | | |
| 239 | 9*H*-Fluorene  | [$C_{13}H_{10}$] [166] | 86-73-7 | 1, 5, 8, 13, 22, 29, 32, 33, 51a, 57, 72a, 97, 113, 114, 124, 126–128, 135, 138, 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*H*-Fluorene, dimethyl- | [$C_{15}H_{14}$] [194] | 30582-01-5 | 22, 294, 392, 400–402, 416, 420–422 |
| 245 | 9*H*-Fluorene, ?,9-dimethyl- | [$C_{15}H_{14}$] [194] | | 416, 420 |
| 246 | 9*H*-Fluorene, 1,9-dimethyl- | [$C_{15}H_{14}$] [194] | 17057-98-6 | 157a, 263, 295, 392 |
| 247 | 9*H*-Fluorene, 2,3-dimethyl- | [$C_{15}H_{14}$] [194] | 4612-63-9 | 157a, 263, 295 |
| 248 | 9*H*-Fluorene, 9,9-dimethyl- | [$C_{15}H_{14}$] [194] | 4569-45-3 | 157a, 263 |
| 249 | 9*H*-Fluorene, dimethylethyl- | [$C_{17}H_{18}$] [222] | 71278-00-7 | 416, 420 |
| 250–251 [b] | 9*H*-Fluorene, ethyl- | [$C_{15}H_{14}$] [194] | 65319-49-5 | 416, 420 |
| 252 | 9*H*-Fluorene, 2-ethyl- | [$C_{15}H_{14}$] [194] | 1207-20-1 | 157a, 263 |
| 253 | 9*H*-Fluorene, 9-ethyl- | [$C_{15}H_{14}$] [194] | 2294-82-8 | 416, 420 |
| 254–255 [b] | 9*H*-Fluorene, ethylmethyl- | [$C_{16}H_{16}$] [208] | 71278-01-8 | 416, 420 |
| A [j] | 9*H*-Fluorene, methyl- | [$C_{14}H_{12}$] [180] | 26914-17-0 | 22, 51a, 124, 239, 388 |
| 256 | 9*H*-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*H*-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*H*-Fluorene, 3-methyl- | [$C_{14}H_{12}$] [180] | 2523-39-9 | 8, 22, 157a, 294, 392, 400–402, 416, 420–422, |
| 259 | 9*H*-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*H*-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*H*-Fluorene, 9-methylene- | [$C_{14}H_{10}$] [178] | 4425-82-5 | 159, 295 |
| 262 | 9*H*-Fluorene, tetramethyl- | [$C_{17}H_{18}$] [222] | 63372-50-9 | 416, 420 |
| 263 | 9*H*-Fluorene, trimethyl- | [$C_{16}H_{16}$] [208] | 30582-02-6 | 416, 420 |
| | *TETRACYCLIC: Benzenoid structures* | | | |
| 264 | Naphthacene  | [$C_{18}H_{12}$] [228] | 92-24-0 | 50, 65, 71, 97, 206, 239, 281, 302, 323, 425, 530 |
| 265 | Benzanthracene, methyl- | [$C_{19}H_{14}$] [242] | 63194-18-3 | 416, 420 |
| 266 | Benz[*a*]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 |
| 267 | Benz[*a*]anthracene, alkyl- | | | 496 |
| 268–269 [b] | Benz[*a*]anthracene, dimethyl- | [$C_{20}H_{16}$] [256] | 43178-07-0 | 71, 341, 400–402, 419-422, 529, 530 |
| 270 | Benz[*a*]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[*a*]anthracene, ethyl- | [$C_{20}H_{16}$] [256] | 31632-62-9 | 71, 216, 336, 529 |
| 272 | Benz[*a*]anthracene, ethylmethyl- | [$C_{21}H_{18}$] [270] | 71265-32-2 | 475 |
| 273 | Benz[*a*]anthracene, methyl- | [$C_{19}H_{14}$] [242] | 43178-22-9 | 239, 398, 401, 402, 419, 421, 422 |
| 274 | Benz[*a*]anthracene, 1-methyl- | [$C_{19}H_{14}$] [242] | 2498-77-3 | 71, 216, 400; 419–422, 530 |
| 275 | Benz[*a*]anthracene, 2-methyl- | [$C_{19}H_{14}$] [242] | 2498-76-2 | 56, 71, 530 |
| 276 | Benz[*a*]anthracene, 3-methyl- | [$C_{19}H_{14}$] [242] | 2498-75-1 | 71, 97, 216, 278, 530 |
| 277 | Benz[*a*]anthracene, 4-methyl- | [$C_{19}H_{14}$] [242] | 316-49-4 | 71, 216, 530 |

**Table 6 (*cont.*)**

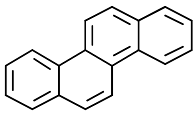
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *TETRACYCLIC: Benzenoid structures (cont.)* | | | |
| 278 | Benz[*a*]anthracene, 5-methyl- | [$C_{19}H_{14}$] [242] | 2319-96-2 | 32, 71, 97, 249, 286, 317, 323, 329, 332, 334, 336, 338, 365, 425, 530 |
| 279 | Benz[*a*]anthracene, 6-methyl- | [$C_{19}H_{14}$] [242] | 316-14-3 | 71, 216; 336, 529 |
| 280 | Benz[*a*]anthracene, 8-methyl- | [$C_{19}H_{14}$] [242] | 2381-31-9 | 71, 216; 336, 529, 530 |
| 281 | Benz[*a*]anthracene, 9-methyl- | [$C_{19}H_{14}$] [242] | 2381-16-0 | 71, 204, 216, 529, 530 |
| 282 | Benz[*a*]anthracene, 10-methyl- | [$C_{19}H_{14}$] [242] | 2381-15-9 | 71, 216, 529, 530 |
| 283 | Benz[*a*]anthracene, 12-methyl- | [$C_{19}H_{14}$] [242] | 2422-79-9 | 71, 475, 365, 529, 530 |
| 284 | Benz[*a*]anthracene, methylene- | [$C_{19}H_{12}$] [240] | | 419 |
| 285 | Benz[*a*]anthracene, propyl- | [$C_{21}H_{18}$] [270] | 71265-33-3 | 216, 529 |
| 286 | Benz[*a*]anthracene, tetramethyl- | [$C_{22}H_{20}$] [284] | | 71, 416, 420, 529 |
| 287–288 [b] | Benz[*a*]anthracene, trimethyl- | [$C_{21}H_{18}$] [270] | 60826-78-0 | 71, 216, 336, 400–402, 416, 420–422, 529, 530 |
| 289 | 7*H*-Benz[*de*]anthracene | [$C_{17}H_{12}$] [216] | 199-94-0 | 24a |




| | | | | |
|---|---|---|---|---|
| 290 | Benzo[*c*]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[*c*]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 |

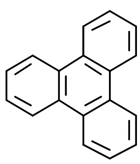


**Table 6 (*cont.*)**

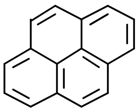
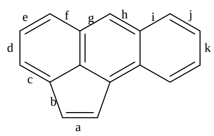
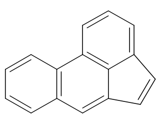
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | | *TETRACYCLIC: Benzenoid structures (cont.)* | | |
| 308 | Triphenylene, dimethyl- | $[C_{20}H_{16}]$ [256] | 60826-76-8 | 400-402, 419-422 |
| 309 | Triphenylene, methyl- | $[C_{19}H_{14}]$ [242] | 41637-89-2 | 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 [l] | 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- | $[C_{20}H_{18}]$ [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 |
| | | *TETRACYCLIC: Cyclopentanoid-benzenoid structures* | | |
| 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.*)**

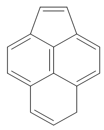
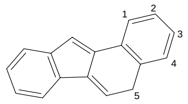
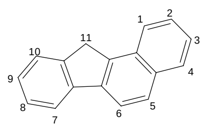
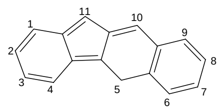
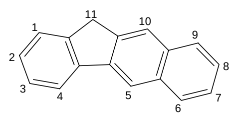
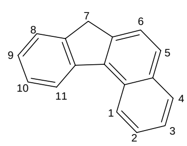
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *TETRACYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | | |
| 347 | Acephenanthrylene, 4,5-dihydro- | [$C_{16}H_{12}$] [204] | 6232-48-0 | 399, 400 |
| 348 | 5*H*-Benz[*fg*]acenaphthylene | [$C_{15}H_{10}$] [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[*a*]fluorene | [$C_{17}H_{12}$] [216] | 30777-18-5 | 51a, 131, 133a, 174, 239a, 323, 474 |
| 361 | 5*H*-Benzo[*a*]fluorene | [$C_{17}H_{12}$] [216] | 238-79-9 | 97, 174, 323, 425 |
| |  | | | |
| 362 | 11*H*-Benzo[*a*]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*H*-Benzo[*a*]fluorene, dimethyl- | [$C_{19}H_{16}$] [244] | | 400, 421, 422 |
| 364 | 11*H*-Benzo[*a*]fluorene, methyl- | [$C_{18}H_{14}$] [230] | 60826-64-4 | 11, 400–402, 419, 421, 422 |
| 365 | 11*H*-Benzo[*a*]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*H*-Benzo[*a*]fluorene, trimethyl- | [$C_{20}H_{18}$] [258] | 71607-85-7 | 400, 416, 420 |
| 369 | 5*H*-Benzo[*b*]fluorene | [$C_{17}H_{12}$] [216] | 243-18-5<br>30777-19-6 | 97, 131, 133a, 174, 239a, 273, 278, 323, 365, 425 |
| |  | | | |
| 370 | 11*H*-Benzo[*b*]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*H*-Benzo[*b*]fluorene, methyl- | [$C_{18}H_{14}$] [230] | 60826-65-5 | 400-402, 419, 421, 422 |
| 372 | 11*H*-Benzo[*b*]fluorene, 9-methyl- | [$C_{18}H_{14}$] [230] | | 419 |
| 373 | Benzo[*c*]fluorene, methyl- | [$C_{18}H_{14}$] [230] | | 416, 420 |
| 374 | 7*H*-Benzo[*c*]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*H*-Benzo[*c*]fluorene, methyl- | [$C_{18}H_{14}$] [230] | 60826-66-6 | 400–402, 416, 420–422 |

**Table 6 (*cont.*)**

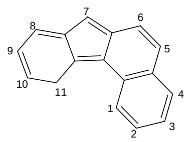
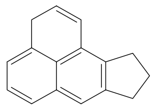
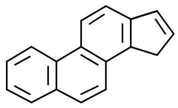
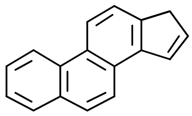
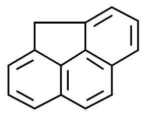
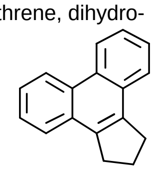
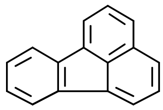
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *TETRACYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | | |
| 376 | 11*H*-Benzo[*c*]fluorene  | $[C_{17}H_{12}]$ [216] | | 174, 379 |
| 377 | Cyclopenta[*a*]phenalene  | $[C_{16}H_{14}]$ [206] | 211-95-0 | 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*H*-Cyclopenta[*a*]phenanthrene  | $[C_{17}H_{12}]$ [216] | 219-07-8 | 97, 323, 520 |
| 383 | 15*H*-Cyclopenta[*a*]phenanthrene, 16,17-dihydro- | $[C_{17}H_{14}]$ [218] | 482-66-6 | 81, 278, 323, 338, 400, 425, 520 |
| 384 | 17*H*-Cyclopenta[*a*]phenanthrene  | $[C_{17}H_{12}]$ [216] | 219-08-9 | 167 |
| 385 | 17*H*-Cyclopenta[*a*]phenanthrene, ethyl- | $[C_{19}H_{16}]$ [244] | 71277-92-4 | 167 |
| 386 | 17*H*-Cyclopenta[*a*]phenanthrene, methyl- | $[C_{18}H_{14}]$ [230] | 71277-93-5 | 167 |
| 387 | 4*H*-Cyclopenta[*def*]phenanthrene  | $[C_{15}H_{10}]$ [190] | 203-64-5 | 131, 196, 197, 198, 278, 323, 342, 398, 419 |
| 388 | 4*H*-Cyclopenta[*def*]phenanthrene, dimethyl- | $[C_{17}H_{14}]$ [218] | 71277-91-3 | 475 |
| 389 | 4*H*-Cyclopenta[*def*]phenanthrene, ethyl- | $[C_{17}H_{14}]$ [218] | 65319-51-9 | 475 |
| 390 | 4*H*-Cyclopenta[*def*]phenanthrene, methyl- | $[C_{16}H_{12}]$ [204] | 58548-39-3 | 475 |
| 391 | Cyclopenta[*l*]phenanthrene, dihydro-  | $[C_{17}H_{14}]$ [218] | | 419 |
| 392 | Fluoraninene, 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.*)**

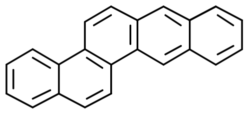
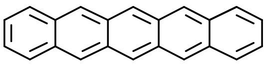
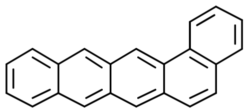
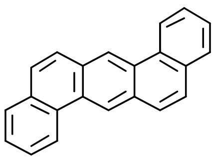
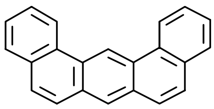
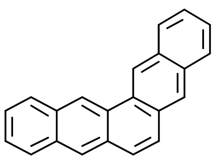
| No. | Polycyclic Aromatic Hydrocarbon | CAS RN | References [a] |
|---|---|---|---|
| | *TETRACYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | |
| 397–399 [b] | Fluoranthene, dimethyl- $[C_{18}H_{14}]$ [230] | 60826-74-6 | 278, 298, 323, 365, 368, 398, 400–402, 419-422, 459 |
| 400 | Fluoranthene, 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 |
| | *PENTACYCLIC: Benzenoid structures* | | |
| 414 | Benzo[*b*]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[*a*]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[*a,h*]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[*a,j*]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.*)**

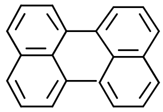
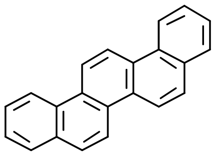
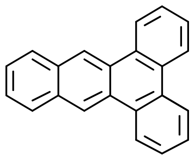
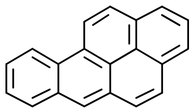
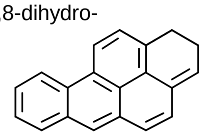
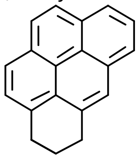
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *PENTACYCLIC: Benzenoid structures (cont.)* | | | |
| 421 | Perylene<br> | $[C_{20}H_{12}]$ [252] | 198-55-0 | 5, 8, 13, 37, 64, 72a, 81, 96, 97, 113, 114, 127, 131, 131a, 133a, 138, 150, 162, 163, 174, 187, 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<br> | $[C_{22}H_{14}]$ [278] | 213-46-7 | 13, 198, 283, 341, 342, 419, 423, 424, 530 |
| 428 | Benzo[*b*]triphenylene<br> | $[C_{22}H_{14}]$ [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[*b*]triphenylene, methyl- | $[C_{23}H_{16}]$ [292] | 64760-20-9 | 419 |
| A [n] | Benzopyrene | $[C_{20}H_{12}]$ [252] | 73467-76-2 | 324, 529 |
| 430 | Benzo[*a*]pyrene<br> | $[C_{20}H_{12}]$ [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[*a*]pyrene, alkyl- | | | 13, 81, 100, 97, 278, 317, 323, 327, 329, 332, 342, 434, 479, 496, 520 |
| 432 | Benzo[*a*]pyrene, 3,4-dihydro- | $[C_{20}H_{14}]$ [254] | | 97, 278, 365, 425 |
| 433 | Benzo[*a*]pyrene, 7,8-dihydro-<br> | $[C_{20}H_{14}]$ [254] | 17573-23-8 | 1, 234a, 278, 323, 338 |
| 434-435 [b] | Benzo[*a*]pyrene, dimethyl- | $[C_{22}H_{16}]$ [280] | 25167-90-2 | 59, 234a, 323, 400, 419, 421, 422, 530 |
| 436 | Benzo[*a*]pyrene, ethyl- | $[C_{22}H_{16}]$ [280] | 71607-83-5 | 475 |
| 437-438 [b] | Benzo[*a*]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*H*-Benzo[*cd*]pyrene, 4,5-dihydro-<br> | $[C_{19}H_{14}]$ [242] | 7130-15-6 | 234a, 400, 419, 421, 422 |

**Table 6 (*cont.*)**

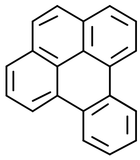
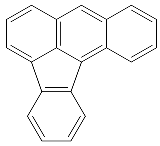
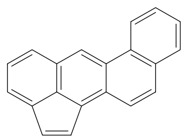
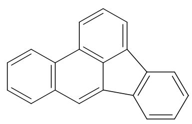
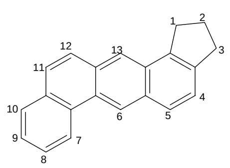
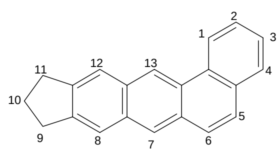
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| 440 | Benzo[*e*]pyrene  | [$C_{20}H_{12}$] [252] | 192-97-2 | 1, 5, 8, 13, 29, 30, 37, 51a, 64, 89, 93, 96, 97, 100, 131, 133, 133a, 137–139, 141, 150, 161, 162, 174, 185, 187, 209, 219, 227, 231, 234a, 239a, 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[*e*]pyrene, dimethyl- | [$C_{22}H_{16}$] [280] | 41699-06-3 | 234a, 400, 419, 421, 422 |
| 443-444 [b] | Benzo[*e*]pyrene, methyl- | [$C_{21}H_{14}$] [266] | 41699-04-1 | 234a, 377, 378, 398, 400-402, 419, 421, 422, 530 |
| 445 | Benzo[*e*]pyrene, trimethyl- | [$C_{23}H_{18}$] [294] | 64760-21-0 | 174, 234a, 419, 448, 451-453 |
| | *PENTACYCLIC: Cyclopentanoid-benzenoid structures* | | | |
| 446 | Benz[*a*]aceanthrylene  | [$C_{20}H_{12}$] [252] | 203-33-8 | 150, 231, 398, 400–402, 419, 421, 422 |
| 447 | Benz[*j*]aceanthrylene  | [$C_{20}H_{12}$] [252] | 202-33-5 | 475, 530 |
| 448 | Benz[*j*]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[*j*]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[*e*]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[*e*]acephenanthrylene, methyl- | [$C_{21}H_{16}$] [266] | 41637-94-9 | 400–402, 419, 421, 422, 530 |
| 452 | Benz[*e*]acephenanthrylene, 10-methyl- | [$C_{21}H_{16}$] [266] | 149021-93-2 | 475 |
| 453 | 1*H*-Benzo[*a*]cyclopent[*h*]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*H*-Benzo[*a*]cyclopent[*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.*)**

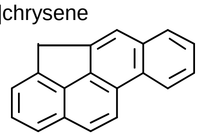
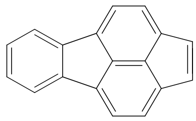
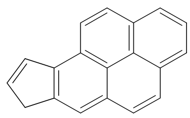
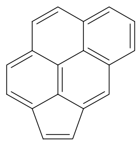
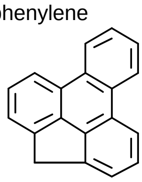
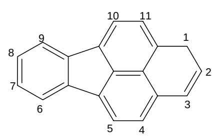
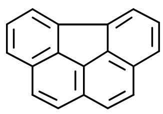
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *PENTACYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | | |
| 455 | 4*H*-Cyclopenta[*def*]chrysene  | $[C_{19}H_{12}]$ [240] | 202-98-2 | 419, 530 |
| 456 | Cyclopenta[*cd*]fluoranthene  | $[C_{18}H_{10}]$ [226] | 193-54-4 | 475 |
| 457 | 1*H*-Cyclopenta[*a*]pyrene  | $[C_{19}H_{12}]$ [240] | 42315-22-0 | 400–402, 419 |
| 458 | Cyclopenta[*a*]pyrene, 3,4-dihydro- | $[C_{19}H_{14}]$ [242] | | 368, 400–402, 419, 421, 422 |
| 459 | Cyclopenta[*a*]pyrene, 3,4-dihydromethyl- | $[C_{20}H_{16}]$ [256] | | |
| 460 | Cyclopenta[*cd*]pyrene  | $[C_{18}H_{10}]$ [226] | 27208-37-3 | 131a, 133a, 234a, 419 |
| 461 | Cyclopenta[*cd*]pyrene, 3,4-dihydro- | $[C_{18}H_{12}]$ [228] | 25732-74-5 | 475 |
| 462 | Cyclopenta[*cd*]pyrene, 3,4-dihydromethyl- | $[C_{19}H_{14}]$ [242] | 64760-18-5 | 475 |
| 463 | 4*H*-Cyclopenta[*def*]triphenylene  | $[C_{19}H_{12}]$ [240] | 23992-32-7 | 419 |
| 464 | Benzofluoranthene | $[C_{18}H_{10}]$ [226] | 56832-73-6 | 5, 216, 417 |
| 465 | Benzofluoranthene, dimethyl- | $[C_{20}H_{14}]$ [254] | | 416, 420 |
| 466 | Benzofluoranthene, ethyl- | $[C_{20}H_{14}]$ [254] | | 216 |
| 467 | Benzofluoranthene, methyl- | $[C_{19}H_{12}]$ [240] | | 416, 420 |
| 468 | 11*H*-Benzo[*cd*]fluoranthene   | $[C_{19}H_{12}]$ [240] | 16135-81-2 | 26, 182, 278, 323, 357, 365, 484, 518 |
| 469 | Benzo[*ghi*]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[*ghi*]fluoranthene, dimethyl- | $[C_{20}H_{14}]$ [254] | 64760-14-1 | 216, 419 |
| 471 | Benzo[*ghi*]fluoranthene, ethyl- | $[C_{20}H_{14}]$ [254] | 71265-35-5 | 475 |
| A [o] | Benzo[*ghi*]fluoranthene, methyl- | $[C_{19}H_{12}]$ [240] | 51001-44-6 | 397, 401, 402, 419, 421, 422 |
| 472 | Benzo[*ghi*]fluoranthene, 1-methyl- | $[C_{19}H_{12}]$ [240] | 71265-21-9 | 216 |
| 473 | Benzo[*ghi*]fluoranthene, 2-methyl- | $[C_{19}H_{12}]$ [240] | 71265-22-0 | 216, 530 |
| 474 | Benzo[*ghi*]fluoranthene, 3-methyl- | $[C_{19}H_{12}]$ [240] | 71265-23-1 | 216, 530 |

**Table 6 (*cont.*)**

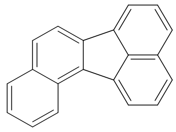
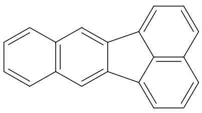
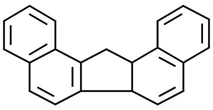
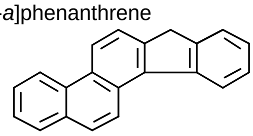
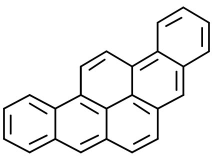
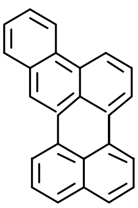
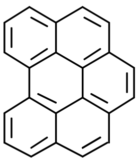
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *PENTACYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | | |
| 475 | Benzo[*ghi*]fluoranthene, 4-methyl- | $[C_{19}H_{12}]$ [240] | 71265-24-2 | 475 |
| 476 | Benzo[*j*]fluoranthene  | $[C_{20}H_{12}]$ [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[*j*]fluoranthene, methyl- | $[C_{21}H_{14}]$ [266] | 60826-67-7 | 419, 421, 422 |
| 478 | Benzo[*k*]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[*k*]fluoranthene, methyl- | $[C_{21}H_{14}]$ [266] | 41637-93-8 | 421, 422, 530 |
| 480 | 13*H*-Dibenzo[*a,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*H*-Indeno[2,1-*a*]phenanthrene  | $[C_{21}H_{14}]$ [266] | 220-97-3 | 34, 97, 278, 323, 338, 342, 351, 353, 425 |
| | *HEXACYCLIC: Benzenoid structures* | | | |
| 482 | Benzo[*rst*]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[*b*]perylene  | $[C_{24}H_{14}]$ [302] | 197-70-6 | 419 |
| 485 | Benzo[*ghi*]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[*ghi*]perylene, dimethyl- | $[C_{24}H_{16}]$ [304] | 64760-22-1 | 419 |
| 489-490 [b] | Benzo[*ghi*]perylene, methyl- | $[C_{23}H_{14}]$ [290] | 41699-09-6 | 8, 400, 419 |
| 491-492 [b] | Benzo[*ghi*]perylene, trimethyl- | $[C_{25}H_{18}]$ [318] | 64760-23-2 | 419 |

**Table 6 (*cont.*)**

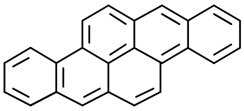
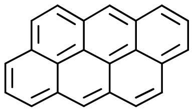
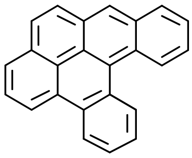
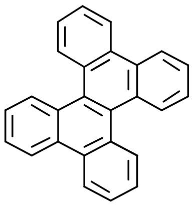
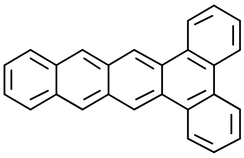
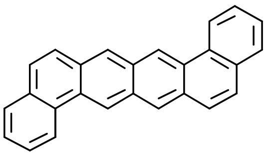
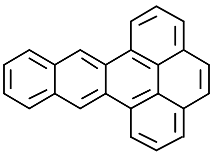
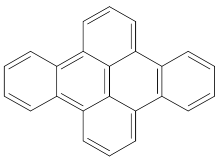
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *HEXACYCLIC: Benzenoid structures (cont.)* | | | |
| 493 | Dibenzo[*b,def*]chrysene  | [$C_{24}H_{14}$] [302] | 189-64-0 | 13, 37, 89, 97, 150, 174, 230, 231, 268, 278, 286, 311, 312, 317, 320, 323, 326, 329, 334, 336, 338, 342, 389, 365, 414, 414a, 417, 419, 423–425, 448–453, 477, 483, 500, 509, 519, 520, 529, 530 |
| 494 | Dibenzo[*def,mno*]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[*def,mno*]chrysene, dimethyl- | [$C_{24}H_{16}$] [304] | 64760-24-3 | 419 |
| 497–499 [b] | Dibenzo[*def,mno*]chrysene, methyl- | [$C_{23}H_{14}$] [290] | 41699-10-9 | 341, 419 |
| 500 | Dibenzo[*def,mno*]chrysene, 6-methyl- | [$C_{23}H_{14}$] [290] | | 460 |
| 501 | Dibenzo[*def,p*]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[*g,p*]chrysene  | [$C_{26}H_{16}$] [328] | 191-68-4 | 24a |
| 503 | Dibenzo[*a,c*]naphthacene  | [$C_{26}H_{16}$] [328] | 216-00-2 | 37, 97, 230, 278, 323, 338, 425 |
| 504 | Dibenzo[*a,j*]naphthacene  | [$C_{26}H_{16}$] [328] | 227-04-3 | 97, 278, 323, 338, 425, 435, 477, 483, 490, 491, 519, 520 |
| 505 | Dibenzo[*de,qr*]naphthacene  | [$C_{24}H_{14}$] [302] | 193-09-9 | 150, 205, 231, 278, 317, 323, 329, 332 , 338 |
| 506 | Dibenzo[*fg,op*]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.*)**

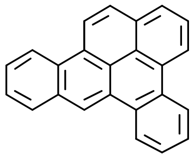
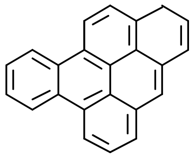
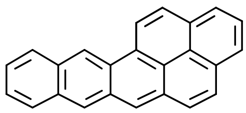
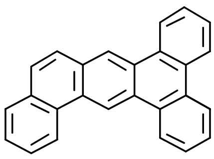
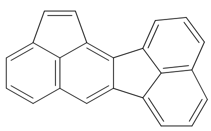
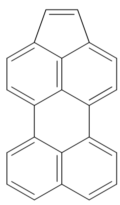
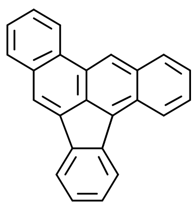
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *HEXACYCLIC: Benzenoid structures (cont.)* | | | |
| 508 | Naphtho[1,2,3,4-*def*]chrysene | $[C_{24}H_{14}]$ [302] | 192-65-4 | 13, 150, 154, 156, 157, 174, 231, 268, 283, 320, 323, 326, 336, 342, 414, 414a, 419, 423, 424, 529, 530 |
| |  | | | |
| 509 | 1*H*-Naphtho[3,2,1,8-*defg*]chrysene | $[C_{23}H_{14}]$ [290] | 190-99-8 | 323, 483 |
| |  | | | |
| 510 | Naphtho[2,1,8-*qra*]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-*b*]triphenylene | $[C_{26}H_{16}]$ [328] | 215-26-9 | 37, 97, 182, 230, 278, 323, 338, 342, 365, 425, 530 |
| |  | | | |
| | *HEXACYCLIC: Cyclopentanoid-benzenoid structures* | | | |
| 512 | Acenaphth[1,2-*a*]acenaphthylene | $[C_{22}H_{12}]$ [276] | 340-99-86 | 216 |
| |  | | | |
| 513 | Acenaphth[1,2-*a*]acenaphthylene, methyl- | $[C_{23}H_{14}]$ [290] | 71265-26-4 | 216 |
| 514 | Cyclopenta[*cd*]perylene | $[C_{22}H_{12}]$ [276] | 189-01-5 | 216 |
| |  | | | |
| 515 | Cyclopenta[*cd*]perylene, methyl- | $[C_{23}H_{14}]$ [290] | | 216 |
| 516 | Dibenz[*a,e*]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.*)**

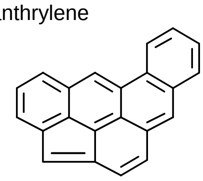
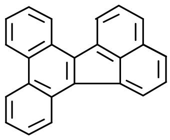
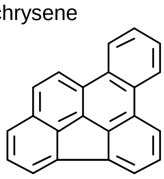
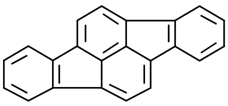
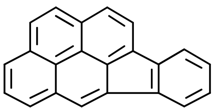
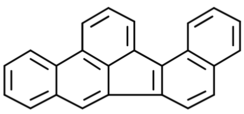
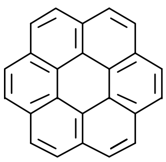
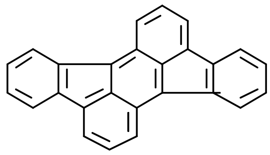
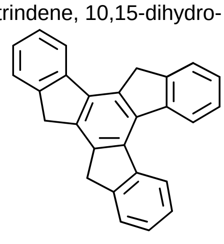
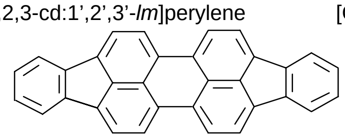
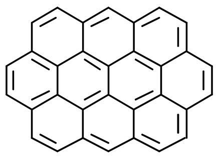
| No. | Polycyclic Aromatic Hydrocarbon | | CAS RN | References [a] |
|---|---|---|---|---|
| | *HEXACYCLIC: Cyclopentanoid-benzenoid structures (cont.)* | | | |
| 517 | Dibenz[*j,mno*]aceanthrylene | [$C_{22}H_{12}$] [276] | 71630-69-8 | 216 |
| |  | | | |
| 518 | Dibenz[*j,mno*]aceanthrylene, methyl- | [$C_{23}H_{14}$] [290] | 71630-69-8 | 216 |
| 519–520 [b] | Dibenzofluoranthene | | 60382-88-9 | 419 |
| 521 | Dibenzo[*j,l*]fluoranthene | [$C_{24}H_{14}$] [302] | 203-18-9 | 416, 420 |
| |  | | | |
| 522 | Indeno[1,2,3,4-*defg*]chrysene | [$C_{22}H_{12}$] [276] | 668-30-4 | 216 |
| |  | | | |
| 523 | Indeno[1,2,3,4-*defg*]chrysene, methyl- | [$C_{23}H_{14}$] [290] | 71277-94-6 | 216 |
| 524 | Indeno[1,2,3-*cd*]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-*cd*]fluoranthene, methyl- | [$C_{23}H_{14}$] [290] | 41699-07-4 | 216 |
| 526 | Indeno[1,2,3-*cd*]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-*cd*]pyrene, dimethyl- | [$C_{23}H_{14}$] [290] | 64158-99-2 | 234a, 419 |
| 529–530 [b] | Indeno[1,2,3-*cd*]pyrene, methyl- | [$C_{23}H_{14}$] [290] | 64158-98-1 | 234a, 419 |
| 531 | Indeno[1,2,3-*cd*]pyrene, trimethyl- | [$C_{25}H_{18}$] [318] | 65140-04-7 | 419 |
| 532 | Naphth[1,2-*e*]acephenanthrylene | [$C_{24}H_{14}$] [302] | 5385-22-8 | 397, 419 |
| |  | | | |
| | *HEPTACYCLIC: Benzenoid structure* | | | |
| 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] |
|---|---|---|---|
| | *HEPTACYCLIC: Cyclopentanoid-benzenoid structure* | | |
| 536 | Rubicene [$C_{26}H_{14}$] [326]  | 197-61-5 | 177, 323, 351, 353 |
| 537 | 5*H*-Tribenzo[*a,f,l*]trindene, 10,15-dihydro- [$C_{27}H_{18}$] [342]  | 27096-03-3<br>548-35-6 | 323, 351–353, 529 |
| | *NONACYCLIC: Cyclopentanoid-benzenoid structure* | | |
| 538 | Diindeno[1,2,3-cd:1',2',3'-*lm*]perylene [$C_{32}H_{16}$] [400]  | 188-94-3 | 351–354 |
| | *DECACYCLIC: Benzenoid structure* | | |
| 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) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *BICYCLIC: Benzenoid structure* | | | | | | | | | | | |
| 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) | Pullman-Pullman (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 |
| 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 |
| 9*H*-Fluorene | 239 | – | – | – | – | – | – | – | – | – | 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) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *TETRACYCLIC: Benzenoid structures* | | | | | | | | | | | |
| Naphthacene | 264 | X | – | – | – | – | X | – | – | – | X |
| Benz[*a*]anthracene | 266 | X | X | – | X | – | X | – | – | – | X |
| Benz[*a*]anthracene, dimethyl- | 268–269 | X[8][d] | – | – | – | – | – | – | – | X[6] | X[23] |
| Benz[*a*]anthracene, 7,12-dimethyl- | 270 | X | – | – | X | – | X | X | X | X | X |
| Benz[*a*]anthracene, ethyl- | 271 | – | – | – | – | – | – | – | – | X[1] | – |
| Benz[*a*]anthracene, 1-methyl- | 274 | X | – | – | – | – | – | – | – | – | X |
| Benz[*a*]anthracene, 2-methyl- | 275 | X | – | – | – | – | – | – | – | – | X |
| Benz[*a*]anthracene, 3-methyl- | 276 | X | – | – | – | – | – | – | – | – | X |
| Benz[*a*]anthracene, 4-methyl- | 277 | X | – | – | – | – | – | – | – | – | X |
| Benz[*a*]anthracene, 5-methyl- | 278 | X | – | – | – | – | – | – | – | X | X |
| Benz[*a*]anthracene, 6-methyl- | 279 | X | – | – | – | – | – | – | – | X | – |
| Benz[*a*]anthracene, 8-methyl- | 280 | X | – | – | – | – | – | – | – | X | X |
| Benz[*a*]anthracene, 9-methyl- | 281 | X | – | – | X | – | – | – | – | X | X |
| Benz[*a*]anthracene, 10-methyl | 282 | X | – | – | – | – | – | – | – | X | X |
| Benz[*a*]anthracene, 12-methyl- | 283 | X | – | – | – | – | – | – | – | X | X |
| Benz[*a*]anthracene, propyl- | 285 | – | – | – | – | – | – | – | – | X[1] | – |
| Benz[*a*]anthracene, tetramethyl- | 286 | X[1] | – | – | – | – | – | – | – | X[2] | – |
| Benz[*a*]anthracene, trimethyl- | 287–288 | X[3] | – | – | – | – | – | – | – | X[3] | X[13] |
| Benzo[*c*]phenanthrene | 290 | X | – | X | – | – | X | – | – | X | X |
| Benzo[*c*]phenanthrene,methyl | 291 | X[4] | – | – | – | – | – | – | – | X[6] | X[6] |
| Chrysene | 292 | X | – | X | X | – | X | – | X | X | X |
| Chrysene, dimethyl- | 294 | – | – | – | – | – | X[1] | – | – | X[1] | X[10] |
| Chrysene, 1-methyl- | 297 | – | – | – | – | – | – | – | – | – | 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) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *TETRACYCLIC: Benzenoid structures (cont.)* | | | | | | | | | | | |
| Pyrene, pentamethyl- | 332–334 | – | – | – | – | X | – | – | – | – | – |
| Pyrene, tetramethyl- | 338–341 | – | – | – | – | X | – | – | – | – | – |
| Pyrene, trimethyl- | 342–344 | – | – | – | – | X | – | – | – | – | – |
| *TETRACYCLIC: Cyclopentanoid-benzenoid structures* | | | | | | | | | | | |
| 7*H*-Benzo[*c*]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 |
| *PENTACYCLIC: Benzenoid structures* | | | | | | | | | | | |
| Benzo[*b*]chrysene | 414 | – | – | X | – | – | X | – | – | – | X |
| Pentacene | 415 | – | – | X | – | – | X | – | – | X | X |
| Benzo[*a*]naphthacene | 416 | – | – | X | – | – | X | – | – | – | X |
| Dibenz[*a,h*]anthracene | 418 | X | X | X | X | – | X | X | – | X | X |
| Dibenz[*a,j*]anthracene | 419 | X | – | X | – | – | X | – | – | X | X |
| Pentaphene | 420 | X | – | – | – | – | X | – | – | – | X |
| Perylene | 421 | – | – | X | – | – | X | – | – | – | X |
| Picene | 427 | – | – | – | – | – | X | – | – | – | – |
| Benzo[*b*]triphenylene | 428 | – | – | X | – | – | X | X | – | X | X |
| Benzopyrene | A[e] | – | – | – | – | – | – | – | – | X | – |
| Benzo[*a*]pyrene | 430 | – | – | X | – | X | X | X | X | X | X |
| Benzo[*a*]pyrene, 7,8-dihydrol- | 433 | – | – | – | – | X | – | – | – | – | – |
| Benzo[*a*]pyrene, dimethyl- | 434–435 | – | – | – | – | X | – | – | – | – | X[9] |
| Benzo[*a*]pyrene, methyl- | 437–438 | – | – | – | – | X | – | – | – | – | X[1] |
| 3*H*-Benzo[*cd*]pyrene, 4,5-dihydro- | 439 | – | – | – | – | X | – | – | – | – | – |
| Benzo[*e*]pyrene | 440 | – | – | X | – | X | X | X | X | X | X |
| Benzo[*e*]pyrene,dimethyl- | 441–442 | – | – | – | – | X | – | – | – | – | – |
| Benzo[*e*]pyrene, methyl- | 443–444 | – | – | – | – | X | – | – | – | – | X[12] |
| Benzo[*e*]pyrene, trimethyl- | 445 | – | – | – | – | X | – | – | – | – | – |
| *PENTACYCLIC: Cyclopentanoid-benzenoid structures* | | | | | | | | | | | |
| Benz[*a*]aceanthrylene | 446 | – | – | X | – | – | – | – | – | – | X |
| Benz[*j*]aceanthrylene, 1,2-dihydro- | 448 | – | – | – | – | – | – | – | – | X | X |
| Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl- | 449 | – | – | – | X | – | X | X | | X | X |
| Benz[*e*]acephenanthrylene | 450 | – | – | X | – | – | – | – | – | X | X |
| Benz[*e*]acephenanthrylene, methyl- | 451 | – | – | – | – | – | – | – | – | – | X[6] |
| 1*H*-Benzo[*a*]cyclopent[*h*]anthracene, 2,3-dihydro- | 453 | 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) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *PENTACYCLIC: Cyclopentanoid-benzenoid structures* | | | | | | | | | | | |
| 9*H*-Benzo[*a*]cyclopent[*i*]anthracene, 10,11-dihydro- | 454 | X | – | – | – | – | – | – | – | – | X |
| 4*H*-Cyclopenta[*def*]chrysene | 455 | – | – | – | – | – | – | – | – | – | X |
| Cyclopenta[*cd*]pyrene | 460 | – | – | – | – | X | – | – | – | – | – |
| Benzo[*ghi*]fluoranthene | 469 | – | – | – | – | – | – | – | – | – | X |
| Benzo[*ghi*]fluoranthene, 2-methyl- | 473 | – | – | – | – | – | – | – | – | – | X |
| Benzo[*ghi*]fluoranthene, 3-methyl- | 474 | – | – | – | – | – | – | – | – | – | X |
| Benzo[*j*]fluoranthene | 476 | – | – | – | – | – | – | – | – | X | X |
| Benzo[*k*]fluoranthene | 478 | – | – | X | – | – | – | – | – | – | X |
| Benzo[*k*]fluoranthene, methyl- | 479 | – | – | – | – | – | – | – | – | – | X[3] |
| 13*H*-Dibenzo[*a,i*]fluorene | 480 | – | – | – | – | – | – | – | – | – | X |
| *HEXACYCLIC: Benzenoid structures* | | | | | | | | | | | |
| Benzo[*rst*]pentaphene | 482 | – | – | X | – | – | – | X | – | X | X |
| Benzoperylene | 483 | – | – | – | – | – | – | – | – | – | – |
| Benzo[*ghi*]perylene | 485 | – | – | X | – | – | – | – | – | X | X |
| Dibenzo[*b,def*]chrysene | 493 | – | – | X | – | – | X | – | – | X | X |
| Dibenzo[*def,mno*]chrysene | 494 | – | – | X | – | – | X | – | – | – | X |
| Dibenzo[*def,p*]chrysene | 501 | – | – | X | – | – | X | – | – | X | X |
| Dibenzo[*a,j*]naphthacene | 504 | – | – | – | – | – | X | – | – | – | – |
| Dibenzo[*de,qr*]naphthacene | 505 | – | – | X | – | – | – | – | – | – | – |
| Dibenzo[*fg,op*]naphthacene | 506 | – | – | X | – | X | X | – | – | – | X |
| Dibenzopyrene | 507 | – | – | – | – | X | – | – | – | – | – |
| Naphtho[1,2,3,4-*def*]chrysene | 508 | – | – | X | – | – | X | – | – | X | X |
| Naphtho[2,1,8-*qra*]naphthacene | 510 | – | – | X | – | – | X | – | – | – | X |
| Naphtho[1,2-*b*]triphenylene | 511 | – | – | X | – | – | X | – | – | – | X |
| *HEXACYCLIC: Cyclopentanoid-benzenoid structures* | | | | | | | | | | | |
| Dibenz[*a,e*]aceanthrylene | 516 | – | – | X | – | – | – | – | – | – | X |
| Indeno[1,2,3-*cd*]pyrene | 526 | – | – | – | – | X | – | – | – | X | X |
| Indeno[1,2,3-*cd*]pyrene, dimethyl- | 527–528 | – | – | – | – | X | – | – | – | – | – |
| Indeno[1,2,3-*cd*]pyrene, methyl- | 529–530 | – | – | – | – | X | – | – | – | – | – |
| *HEPTACYCLIC: Benzenoidstructure* | | | | | | | | | | | |
| Coronene | 533 | – | – | X | – | – | – | – | – | X | X |
| *HEPTACYCLIC: Cyclopentanoid-benzenoid structure* | | | | | | | | | | | |
| 5*H*-Tribenzo[*a,f,l*]trindene, 10,15-dihydro- | 537 | – | – | – | – | – | – | – | – | X | – |
| *DECACYCLIC: Benzenoidstructure* | | | | | | | | | | | |
| 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 potently 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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