

PREPARATION AND INFRARED SPECTRA OF ANTHRACENE, ITS METHYL DERIVATIVES AND SOME OTHER LINEAR POLYNUCLEAR HYDROCARBONS

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The infrared spectra were measured of solid samples of anthracene and its 2-methyl-, 2,3-, 2,6-, 2,7-dimethyl-, 2,3,6-trimethyl- and 2,3,6,7-tetramethyl derivatives, naphthacene and its 1,2,3,4-tetrahydro derivative, and pentacene. These hydrocarbons were prepared by reducing appropriate quinones with aluminium tri(cyclohexyl oxide). Absorption bands of characteristic vibrations were found and interpreted.

Many authors¹⁻¹⁰ studied infrared spectra of polynuclear aromatic hydrocarbons, some of them tried to correlate their own results with those of studies of differently substituted benzene derivatives. Especially, the region of CH out-of-plane deformation vibrations was studied, but some papers involved also the combination and overtone frequency regions⁴⁻⁶. The region of CH stretching vibrations of higher polynuclear hydrocarbons was also investigated^{2,3}. In some cases, the substitution type of polynuclear hydrocarbons could be determined, which was considerably more difficult in other cases and even impossible⁸ for compactly condensed hydrocarbons (*e.g.* pyrene). Califano¹ studied infrared spectra of anthracene and some of its derivatives in detail and was engaged in the interpretation of absorption bands in the whole region of infrared spectrum.

Especially this study was taken into consideration in the present paper, and we extended it by involving some methylanthracenes and higher linearly fused polynuclear aromatic hydrocarbons. We have measured infrared spectra of anthracene, 2-methylanthracene, 2,3-, 2,6-, 2,7-dimethylanthracenes, 2,3,6-trimethylanthracene, 2,3,6,7-tetramethylanthracenes, naphthacene, 1,2,3,4-tetrahydronaphthacene, and pentacene. All these hydrocarbons are easily obtainable by the reduction of corresponding quinones by means of aluminium tri(cyclohexyloxyde)¹¹⁻¹⁵.

EXPERIMENTAL

Preparation of Aromatic Hydrocarbons

A mixture of 7.5 ml cyclohexyl alcohol, purified by a column distillation, 375 mg aluminium shavings, 0.2 ml dry tetrachloromethane and 10 mg mercuric chloride was heated to boil under a reflux condenser provided with a silica gel closure. When the mixture began to boil vigorously, it was removed from the bath and kept to react. After the reaction subsided, the mixture was heated to boil for about 2–3 hours, till all aluminium was dissolved. Into the aluminium tri-(cyclohexyloxyde) solution prepared in such a way, 3.6 mmol quinone (2.2 mmol only in case of pentacene-6,13-dione) was added and the mixture was heated to boil under reflux for 4 hours with the exclusion of the air moisture. As a rule, solid hydrocarbon began to appear in the reaction mixture already after a 2 hour reaction. With the exception of anthracene, the hydrocarbons were separated in the following way. The cooled reaction mixture was mixed with an equal volume of acetic acid, diluted with 2-fold volume of methyl alcohol, and kept at room temperature for 1 h. Solid hydrocarbon was then filtered, washed with methyl alcohol, 10% HCl, water, and again with methyl alcohol, and dried in air at 50°C. The yields were 47–76%. Methylated anthracenes were purified by means of crystallization from benzene and, in some cases, by sublimation *in vacuo* in the carbon dioxide flow. Pentacene and naphthacene were also purified by this method, the latter being crystallized also from dimethylformamide. Anthracene, which is soluble in alcohols to a great extent, was separated from the reaction mixture by an extraction with benzene and following steam stripping¹¹ of the solvents. Ethyl alcohol was used for the crystallization of anthracene. The characteristics of the samples prepared are summarized in Table I. The melting points were determined in a capillary and were not corrected.

TABLE I
Characterization of Polynuclear Hydrocarbons Studied

Compound	M.p., °C ^a (ref.)
Anthracene (<i>I</i>)	213/213–216 (18)
2-Methylanthracene (<i>II</i>)	207/206–207 (19)
2,3-Dimethylanthracene (<i>III</i>) ^c	253/252 (20)
2,6-Dimethylanthracene (<i>IV</i>)	248/250 ^b (21)
2,7-Dimethylanthracene (<i>V</i>)	241/241 ^b (21)
2,3,6-Trimethylanthracene (<i>VI</i>)	253/255 ^b (22)
2,3,6,7-Tetramethylanthracene (<i>VII</i>)	301/301 (23)
Naphthacene (<i>VIII</i>)	350/350–351 (15)
1,2,3,4-Tetrahydronaphthacene (<i>IX</i>)	237/236–237 (15)
Pentacene (<i>X</i>)	— ^c (13, 14)

^a The first value was obtained by the authors, the second one was taken from literature (with references in parentheses); ^b values from literature with a correction; ^c no melting point, only sublimation.

Measurement of Infrared Spectra

The infrared spectra were measured with a Beckmann IR-7 double-beam grating spectrophotometer working in two main regions: 200–650 and 600–4000 cm^{-1} . As the hydrocarbons studied, with exception of lower members of the series, are insoluble in common solvents used in the spectroscopy, the technique of KBr pellets was used for measurements. All compounds were measured in the solid phase to enable a comparison of the spectra of individual compounds. The concentrations of about 3 mg sample/300 mg KBr or 1 mg sample/300 mg KBr were used. The wavenumbers of infrared bands of all compounds studied are presented in Table II.

RESULTS AND DISCUSSION

All spectra were measured as KBr pellets and show a medium intense, broad band due to the absorbed humidity near 3460 cm^{-1} . Dry pellets were seldom obtained on drying over P_2O_5 *in vacuo*.

In the infrared spectra of polynuclear aromatic hydrocarbons, the bands of modes belonging to the motions of skeletal C atoms as well as of H atoms attached are assigned. In many cases, spectral properties of polynuclear hydrocarbons did not differ from general properties of aromatic hydrocarbons; let us show important patterns of their spectra in more detail.

CH Stretching Vibrations

On examining wavenumbers of the strongest band in the region of CH stretching vibrations of anthracene (3056 cm^{-1}), naphthalene (3047 cm^{-1}), and pentacene (3051 cm^{-1}), the previously described correlation² (a systematic decrease in the wavenumber with increasing number of rings) was not proved. On the other hand, the appearance of CH stretching region in the spectra of methyl derivatives of anthracene agrees well with those published earlier² or found in the spectra of benzenanthracene methyl derivatives³. In general, the CH stretching region seems to become simpler when the number of rings increases. *E.g.* anthracene shows six absorption bands between 3085 and 2955 cm^{-1} while pentacene only three bands.

CH Bending Vibrations

As expected, rather intense bands of the in-plane bending vibrations of aromatic hydrogens occur between 1280 and 990 cm^{-1} . This seems to be a specific peculiarity of polynuclear hydrocarbons; the intensities of bands of analogous vibrations in the spectra of simpler aromatic compounds are rather weak when not enhanced by the interaction with a substituent (*e.g.* with a carbonyl group¹⁶).

The bands of out-of-plane vibrations of aromatic hydrogens were observed in the range of 960 – 720 cm^{-1} . The spectra of polynuclear hydrocarbons show many intense bands of the out-of-plane vibrations and even more bands if their skeleton becomes compact⁸ (when it shares more than two C—C bonds with other cycles).

TABLE II
Vibrational Assignment of Polynuclear Hydrocarbons I-X

Vibrational assignment	I	II	III	IV	V	VI	VII	VIII	IX	X
Region of CH stretch bands										
CH stretch arom.	3 085 w	3 098 w	3 090 w	—	—	—	—	3 084 sh	3 080 sh	3 081 sh
CH stretch arom.	3 056 s	3 054 s	3 054 s	3 056 m	3 055 w	3 054 w	3 056 vw	3 062 sh	3 051 s	3 051 s
CH stretch arom.	—	—	—	3 034 sh	3 033 sh	3 022 sh	3 019 sh	3 047 s	—	—
CH stretch arom.	3 028 m	3 031 m	3 026 m	3 022 m	3 019 m	3 012 m	3 012 s	3 034 sh	3 026 sh	3 026 sh
CH stretch arom.	3 015 sh	3 013 sh	3 014 sh	—	—	—	—	3 006 sh	3 011 sh	—
CH stretch arom.	2 990 w	—	—	—	—	—	—	—	—	—
CH stretch assym. CH ₃	—	2 985 w	2 984 m	2 981 m	2 975 m	2 983 s	2 985 s	2 977 vw	—	—
CH stretch	2 955 sh	—	—	—	—	—	—	2 955 vw	—	—
CH stretch	—	2 938 m	2 936 s	2 923 sh	2 926 sh	2 935 s	2 941 s	—	—	—
CH stretch	—	—	—	—	—	—	—	—	2 936 vs	—
CH stretch	2 925 m	—	—	—	—	—	—	—	—	2 925 m
CH stretch	—	2 915 m	2 915 m	2 912 s	2 910 s	2 917 s	2 919 s	—	—	—
CH stretch	2 915 sh	—	—	—	—	—	—	—	—	—
CH stretch	2 872 sh	2 898 sh	2 895 sh	—	2 895 sh	2 894 sh	—	2 901 vw	2 875 sh	—
CH stretch	—	—	2 880 sh	—	—	—	—	—	—	—
CH stretch CH ₃ sym.	—	2 865 w	2 851 w	2 863 m	2 865 m	2 865 sh	2 888 sh	—	—	2 854 w
CH stretch sym. CH ₂	—	—	—	—	—	—	—	—	2 859 s	—
CH stretch	2 853 vw	2 845 sh	2 800 sh	2 846 w	2 846 sh	—	2 847 sh	—	2 838 sh	—
CH stretch	2 823 sh	—	—	—	—	—	2 757 vw	—	2 798 sh	—
CH stretch	—	2 732 w	2 735 w	2 728 w	2 725 w	2 730 w	2 731 w	—	2 663 w	—
CH stretch	2 530 vw	2 530 vw	—	—	—	—	—	—	2 653 sh	—
CH stretch	2 440 vw	2 438 vw	—	—	—	—	2 475 vw	—	—	—
CH stretch	2 312 vw	2 330 vw	—	—	—	—	2 200 vw	—	—	—

Region of overtone and combination tone bands

1 950 w	1 942 sh	—	—	—	—	1 943 w	—	1 948 w
1 931 w	1 928 w	1 934 w	1 924 w	1 922 w	1 920 w	1 926 w	1 935 w	1 930 sh
1 915 vw	—	1 923 w	—	—	—	—	1 917 vw	—
—	—	—	—	—	—	—	1 903 vw	—
1 860 vw	1 860 vw	1 857 vw	1 868 vw	—	—	1 867 vw	—	—
—	—	—	1 833 vw	—	—	1 838 vw	1 828 w	—
1 808 w	1 808 w	1 804 m	1 808 w	1 815 vw	1 811 m	1 806 m	1 800 w	1 810 w
—	1 797 sh	—	—	—	—	—	—	1 802 sh
1 787 w	1 787 w	—	1 771 w	1 785 w	—	—	1 791 sh	—
—	1 764 vw	—	—	1 771 w	—	—	1 761 vw	1 765 w
—	—	—	1 751 sh	—	1 759 w	—	1 734 sh	—
1 726 w	1 736 vw	1 725 w	1 735 w	—	—	1 736 w	1 726 w	—
1 701 w	1 705 w	—	—	1 713 vw	1 710 w	1 712 vw	1 707 sh	1 713 sh
—	—	—	—	—	—	—	1 705 vw	—
—	1 670 w	1 696 w	1 672 sh	1 658 sh	1 695 w	1 682 w	1 681 vw	1 699 sh
—	—	1 662 sh	—	—	—	—	—	1 677 s

Region of ring stretching bands

1 653 sh	1 648 sh	—	—	—	1 654 sh	1 653 sh	—	1 655 sh	1 668 sh
1 638 sh	—	1 648 sh	—	—	1 644 sh	1 648 sh	—	1 648 sh	1 637 sh
1 623 s	1 639 s	1 634 m	1 636 s	1 636 s	1 636 s	1 644 s	1 637 sh	—	1 630 s
—	—	1 629 sh	1 621 sh	—	—	—	—	—	—
—	1 635 sh	—	—	—	—	—	1 632 m	1 630 m	1 624 sh
—	1 627 sh	1 623 sh	—	—	1 620 sh	1 635 sh	1 602 sh	—	—
—	—	—	—	—	—	1 618 sh	—	—	—
—	1 605 w	—	—	—	—	1 600 sh	—	—	1 601 s
—	1 587 sh	1 588 w	—	1 588 w	1 594 w	1 584 sh	—	1 583 vw	1 583 sh
—	—	—	—	—	—	1 566 vw	—	—	—
1 570 vw	1 556 sh	1 543 sh	—	—	—	—	—	—	—
—	1 547 sh	—	—	—	—	—	—	1 544 sh	1 544 w
1 538 m	1 539 m	1 539 m	1 540 m	1 541 m	1 534 m	1 532 m	1 542 m	1 532 m	—

TABLE II
(Continued)

Vibrational assignment	I	II	III	IV	V	VI	VII	VIII	IX	X
	—	1 533 sh	—	—	—	—	—	—	—	—
	1 497 sh	1 508 sh	1 533 sh	1 523 sh	—	—	—	1 505 vw	1 490 sh	—
Ring stretch	—	—	1 500 sh	—	1 487 w	1 492 sh	1 512 sh	—	1 479 sh	1 503 m
	1 481 w	1 483 sh	1 491 sh	—	—	—	1 493 sh	—	—	—
Ring stretch	—	—	1 480 m	—	—	—	—	—	—	1 475 sh
	1 459 s	—	1 461 s	1 474 m	—	1 470 s	1 464 s	1 466 s	—	1 459 m
CH deform. assym. CH ₃	—	1 463 m	1 456 s	1 460 m	1 463 s	1 455 s	1 469 s	—	—	—
	—	1 458 sh	—	—	1 459 sh	—	—	—	—	—
CH ₂ scissor	—	—	—	—	—	—	—	—	1 461 s	—
	—	—	—	—	—	—	—	—	1 458 sh	—
Ring stretch	1 454 s	—	—	—	—	—	1 456 s	—	1 446 sh	—
Ring stretch	—	—	—	—	—	—	1 448 sh	—	1 438 m	1 448 m
	1 448 sh	1 448 sh	1 447 sh	1 449 sh	1 443 sh	1 436 sh	1 437 sh	—	1 435 m	—
	1 424 w	1 412 vw	1 430 w	—	—	1 414 w	1 417 m	1 410 sh	—	1 418 w
	—	—	1 406 w	1 400 sh	—	—	1 392 sh	—	1 402 w	—
Ring stretch	1 401 w	—	—	—	—	—	—	1 389 m	1 387 sh	1 396 m
	1 380 sh	—	—	—	—	—	—	—	—	1 387 sh
CH def. sym. CH ₃	—	1 380 m	1 365 m	1 378 m	1 379 m	1 383 m	1 380 m	—	—	—
	1 349 vw	1 365 vw	—	1 347 vw	1 323 sh	—	1 374 sh	1 331 w	1 365 w	1 356 sh
	—	1 342 w	—	—	—	—	—	—	1 352 w	1 345 m
Ring stretch	—	—	—	—	—	1 343 w	1 326 w	—	1 341 vw	—
	—	—	1 350 m	—	—	1 322 w	—	—	1 321 vw	1 327 w
Ring stretch	1 318 s	1 308 m	1 293 m	1 305 m	1 310 m	1 294 m	1 293 m	1 298 s	1 292 s	1 298 s
	1 286 w	1 293 sh	—	—	—	—	—	1 292 sh	1 282 sh	—
	—	—	—	—	—	—	—	1 285 sh	—	—

Region of CH in-plane bending
bands

1 273 m	1 272 m	1 273 m	1 273 m	1 278 w	1 268 w	1 250 m	1 281 m
1 245 w	1 248 vw	1 245 vw	1 197 w	1 266 w	1 248 sh	1 242 sh	1 253 m
1 221 w	1 225 vw	1 320 sh	—	1 242 vw	—	1 218 vw	—
1 188 sh	1 190 w	1 201 w	—	1 202 w	—	—	1 222 w
—	—	1 198 sh	—	—	—	—	—
—	—	1 188 vw	—	1 192 sh	1 203 s	1 198 w	1 190 m
1 167 m	1 173 m	1 167 m	1 174 m	1 172 w	—	1 164 m	1 163 m
—	1 166 m	—	1 162 sh	—	—	—	—
—	1 154 w	—	—	—	—	1 163 m	—
1 146 s	1 137 w	1 138 vw	1 139 w	1 134 w	—	1 136 sh	1 148 sh
1 126 w	1 111 vw	1 121 m	—	1 119 m	1 106 s	1 126 m	1 118 m
1 119 sh	—	1 112 sh	—	—	1 100 sh	—	1 122 sh
1 075 vw	—	1 065 sh	—	—	—	1 075 w	—
—	—	—	—	—	—	1 067 w	—
1 037 w	—	—	—	1 034 sh	—	—	—
998 s	1 037 m	1 025 s	1 041 m	1 040 m	1 028 s	—	—
—	1 008 m	1 007 s	1 012 vw	1 016 w	—	—	1 018 w
979 w	—	—	—	1 004 m	999 s	995 m	991 m

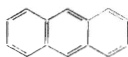
Region of CH-out-of-plane bending
and skelet. defor. bands resp.

957 s	960 sh	—	—	—	968 vw	—	—
—	954 s	953 s	963 s	958 m	—	957 s	958 s
—	947 sh	—	942 m	943 w	—	—	952 s
906 m	—	—	—	—	—	—	—
—	903 sh	—	—	—	—	932 w	—
—	897 sh	—	—	916 s	—	—	—
—	—	—	—	911 sh	—	—	—
886 vs	892 vs	902 vs	905 vs	896 vs	912 vs	905 vs	907 vs
—	—	879 vw	—	—	907 sh	—	890 m
—	868 s	—	873 s	—	905 vs	909 m	—
—	—	—	—	883 w	899 sh	892 vs	—
—	—	—	861 m	865 vw	880 w	—	—

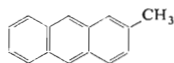
TABLE II
(Continued)

Vibrational assignment	I	II	II	III	V	VI	VII	VIII	IX	X
CH out-of-plane-bending	859 w	---	---	834 vw	810 sh	848 vw	880 m	---	---	---
	---	---	---	793 s	791 vs	795 s	854 vw	---	876 sh	---
	---	802 s	---	---	---	---	834 w	835 vw	852 vw	842 sh
	810 vw	---	---	786 sh	771 m	766 w	790 vw	---	838 w	836 m
	775 m	---	---	771 vw	766 sh	---	770 vw	754 sh	812 w	---
757 w	---	---	---	---	---	---	---	779 vw	794 vw	
---	---	---	---	---	---	---	---	---	767 vw	764 sh
Skelet deform.	743 m	---	---	---	---	---	---	750 sh	---	742 sh
CH out-of-plane bending	737 m	740 vs	741 vs	---	---	---	---	743 vs	742 vs	733 vs
CH out-of-plane bending	729 vs	---	---	---	---	---	---	---	---	---
Region of skelet deform.	---	---	---	---	---	---	734 w	---	---	---
	---	715 sh	---	---	---	---	713 w	717 w	---	714 m
	655 w	648 vw	629 vw	650 vw	646 vw	629 w	---	---	648 vw	629 sh
	---	622 vw	---	---	---	---	---	625 w	637 vw	622 w
	---	---	---	---	---	---	---	---	624 w	---
613 m	---	606 w	---	---	605 w	600 vw	609 w	---	---	
602 s	593 s	---	---	600 s	---	---	---	---	588 vw	
574 vw	581 vw	587 w	---	585 vw	565 m	558 m	558 m	576 vw	580 w	572 w
---	---	---	---	---	---	550 s	---	553 w	---	562 w
---	520 w	---	543 s	549 vw	543 w	---	---	---	---	539 w
---	---	---	525 vw	---	---	---	---	---	---	508 vw
---	---	---	---	---	---	---	---	---	482 sh	477 sh
476 vs	476 vs	477 vs	476 vs	478 vs	476 s	476 s	478 s	472 s	472 s	470 vs

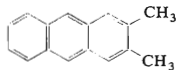
466 s	464 s	468 s	463 s	465 s	466 s	473 sh	460 s	466 sh	455 s
452 w	—	—	—	—	—	414 s	—	—	—
440 sh	390 w	403 s	391 m	402 m	404 s	401 sh	—	440 vw	—
—	—	—	363 w	336 w	377 vw	363 vw	—	406 m	—
—	—	—	—	—	—	—	—	332 m	—
—	326 w	327 m	—	—	325 m	—	—	—	—
—	—	323 sh	—	—	—	—	—	—	—
—	319 sh	—	—	—	—	287 m	—	303 w	—



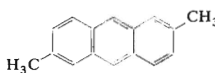
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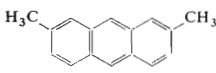
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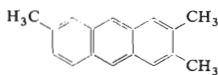
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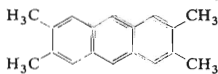
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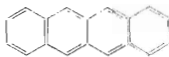
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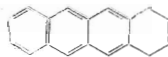
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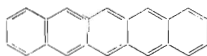
VII



VIII



IX



X

Owing to the fact that the infrared spectrum in the region discussed is rather complex for diagnostical purposes, the absence of a band is at least as useful as its presence⁶. The intensities of infrared bands of the out-of-plane CH vibrations are affected by coupling with ring puckering modes; this effect was described in case of simpler aromatic compounds¹⁷.

It is rather easy for linear polynuclear aromatic hydrocarbons to derive the substitution type from infrared spectrum if one ring (ending the molecule) is substituted only. The substitution of both end rings makes the diagnosis more difficult but the situation never becomes do troublesome as in case of compact polynuclear hydrocarbons like pyrene⁸.

The infrared spectra of polynuclear hydrocarbons show very strong bands of the out-of-plane vibrations of "isolated" hydrogens; the wavenumbers of these bands rise with increasing number of rings from 886 cm^{-1} in anthracene to 907 cm^{-1} in pentacene; if substituting these hydrogens with any substituent, these bands disappear (the substitution in positions 9 and 10 of anthracene^{9,10}).

Some bands in the infrared spectra of polynuclear aromatic hydrocarbons show correlation field splitting^{1,9} when measured in KBr pellets. The band of out-of-plane bending CH vibration of anthracene near 729 cm^{-1} (CS_2 solution) gives a doublet with branches at 737 and 729 cm^{-1} . Naphthacene shows an analogous doublet at 750 and 743 cm^{-1} as well as pentacene at 742 and 733 cm^{-1} . As expected, this splitting is strongly dependent on the structure of crystal cell and therefore it was not found in the spectra of some other substances of this series.

In contradistinction of simple benzenoid hydrocarbons, where region of overtone/composition frequencies, arising from the out-of-plane fundamentals is very useful in structural diagnosis, an analogous region in the spectra of polynuclear hydrocarbons is useless owing to its complexity.

Vibrations of the Heavy Skeleton

With respect to aromatic character of polynuclear hydrocarbons studied, some bands occur in regions where also simple aromatic compounds absorb. Thus, absorption bands in the regions 1650 – 1600 (somewhat broader than those for benzene series, owing to the fixation of unequal C—C bond-lengths) and 1525 – 1475 cm^{-1} are then observed. The wavenumber near 1600 cm^{-1} is somewhat sensitive to a substitution of the hydrocarbon. *E.g.* in anthracene series, the band maximum shifts to higher wavenumbers with increasing number of substituents; the highest value (1644 cm^{-1}) was found in the spectrum of 2,3,6,7-tetramethyl derivative. The bands of ring deformation modes below 700 cm^{-1} are also present in the spectra of polynuclear hydrocarbons. Let us say that the effect of correlation field splitting was there also ascertained; *e.g.* anthracene shows a doublet at 476 and 466 cm^{-1} .

Comments to the Spectra of Linear Polynuclear Hydrocarbons

On the basis of the analysis of vibrational spectrum of anthracene, carried out by Califanol, it is possible to assign some bands from the spectra of naphthacene and pentacene per analogiam to certain vibrational modes (Table III).

Vibrations of the Methyl Groups

Though it is not very easy to find the absorption bands of stretching vibrations of hydrogens situated in the methyl groups,* there are some regions of their probable occurrence. A band of one antisymmetric vibration was found between 2985–2975 cm^{-1} , the band of the symmetric vibration near 2865 cm^{-1} . The bands of the CH_3 deformation vibrations were found near 1460 and 1380 cm^{-1} , as expected.

TABLE III
Vibrational Assignment of Anthracene, Naphthacene and Pentacene

Type of vibration	Species	<i>I</i> ^a	<i>VIII</i>	<i>X</i>
CH out-of-pl. bending		957 s	957 s	958 s
CH out-of-pl. bending		886 vs	905 vs	907 vs
CH out-of-pl. bending	B_{1u}	729 vs	743 vs	733 vs
Skeletal deform.		602 s	—	—
Skeletal deform.		476 vs	472 s	470 vs
CH stretching		3 056 s	3 047 s	3 051 ^s s
Ring stretching		1 623 s	1 632 m	1 630 s
Ring stretching	B_{2u}	1 318 s	1 298 s	1 298 s
CH in pl. bending		1 273 m	—	—
CH in pl. bending		1 146 s	—	—
Skeletal deform.		906 m	—	—
Skeletal deform.		743 m	—	—
Ring stretching		1 538 m	1 542 m	1 544 w
Ring stretching		1 459 s	1 466 s	1 459 m
CH in pl. bending	B_{3u}	1 167 m	1 164 m	1 163 m
CH in pl. bending		998 s	—	—
Skeletal deform.		613 m	—	—

^a Among the data for anthracene, the bands detected by the authors during the study of anthracene single crystal are not given as they are missing in the spectrum of anthracene in KBr pellet.

* In the region between 3000–2800 cm^{-1} , the harmonic/combination bands, originating from lower fundamentals, occur.

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