Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. II. Pyrene Series, Naphthopyrene Series, and Coronene Series

Robert A. Alberty, Michael B. Chung, and Andrea K. Reif

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Received November 2, 1987; revised manuscript received June 28, 1988

The tables in our first paper on polycyclic aromatic hydrocarbons [J. Phys. Chem. Ref. Data 17, 241 (1988)] have been extended by calculating thermodynamic properties for the first four isomer groups in the pyrene series, the first three isomer groups in the naphthopyrene series, and the first three isomer groups in the coronene series. Successive isomer groups in each series differ by C_4H_2. Since chemical thermodynamic properties are known for only a limited number of polycyclic aromatic hydrocarbons, the properties of individual species have been estimated using Benson group values of Stein and Fahr for temperatures from 298.15 to 3000 K. Values of C°_p, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ have been calculated in joules for a standard state pressure of 1 bar. The chemical thermodynamic properties of the individual species have also been calculated. The isomer group values provide a basis for extrapolating to higher carbon numbers where it is not feasible to consider individual molecular species.

Key words: polycyclic aromatic hydrocarbons; pyrene; naphthopyrene; coronene; Benson method; enthalpy of formation; heat capacity; isomer group thermodynamic properties; isomer mole fractions; thermodynamic properties.

Contents

List of Tables

I. Introduction

The preceding article in this series[1] presented thermodynamic tables for the benzene series isomer groups from C_6H_6 to $C_{26}H_{16}$ and for the individual species. This paper extends these tables to the next three isomer groups. Some of the needs for thermodynamic properties of polycyclic aromatic hydrocarbons have been indicated in the preceding article.

Dias[2–6] has developed a formula periodic table for benzenoid polycyclic aromatic hydrocarbons using graph theoretical principles. Molecular formulas in this periodic table represent isomer groups. In thinking about the chemical thermodynamic properties of polycyclic aromatic hydrocarbons it is convenient to think of them in terms of series of isomer groups in which successive isomer groups differ by C_4H_2. Table 1 gives the molecular formulas, numbers of rings, and numbers of isomers for the first four series. In the paper on the benzene series, we found that the thermodynamic properties of the higher isomer groups can be estimated by linear extrapolation from the properties of lower isomer groups. This paper is concerned with the pyrene, naphthopyrene, and coronene series. There is an infinite number of these series, and each has an infinite number of isomer groups.

The numbers of isomers in Table 1 come from Trinajstić and co-workers.[7] We are indebted to them for the computer generation of all the possible structures that correspond to these molecular formulas. The structural formulas of the isomers considered in this paper are given in Fig. 1. To simplify this figure only sigma bonds are shown. However, the thermodynamic properties of all these isomers are not estimated in this paper for the following reasons: (i) Some of the structures are diradicals, and we do not currently know how to estimate their properties—although they are expected to be unstable with respect to the nonradical isomers. (ii) Some of the structures are helicenes in the sense that the hydrogen atoms overlap in the bay region, and this prevents them from being planar molecules; again we do not currently know how to estimate their properties—although they are expected to be unstable with respect to the nonradical isomers.

Table 2 gives the numbers of diradicals for the various isomer groups considered in this paper; they are identified in Trinajstić's tables by $K = 0$, since they do not have any Kekule structures. The identification numbers of the diradical isomers in Fig. 1 are as follows:

$C_{24}H_{14}$	13
$C_{28}H_{16}$	22,51,57,58,66,67
$C_{22}H_{12}$	2
$C_{26}H_{14}$	9
$C_{30}H_{16}$	27,47,53,54,55,56,64,65,66
$C_{28}H_{14}$	8
$C_{32}H_{16}$	15,25,41,44,45,46,48,53,54.

Table 2 also gives the numbers of helicenes that are omitted in the thermodynamic tables. Their identification numbers are as follows:

$C_{28}H_{16}$	3,24,35,36,41,42,48,57
$C_{30}H_{16}$	41,42.

The omission of diradicals and helicenes is not expected to affect the isomer group thermodynamic properties because these species have significantly higher standard Gibbs energies of formation, and therefore do not contribute significantly to the equilibrium population. The tables presented here are of the same type as those published earlier for alkanes,[8] alkylbenzenes,[9] alkenes,[10] alkylnaphthalenes,[11] alkylcyclopentanes and cyclohexanes,[12] alkynes,[13] thiols,[14] alkanols,[15] and benzene-series polycyclic aromatic hydrocarbons.[1]

TABLE 1. First four series of polycyclic aromatic hydrocarbons[a]

N_C	Benzene series	Pyrene series	Naphthopyrene series	Coronene series
6	C_6H_6(1,1)			
8				
10	$C_{10}H_8$(2,1)			
12				
14	$C_{14}H_{10}$(3,2)			
16		$C_{16}H_{10}$(4,1)		
18	$C_{18}H_{12}$(4,5)			
20		$C_{20}H_{12}$(5,3)		
22	$C_{22}H_{14}$(5,12)		$C_{22}H_{12}$(6,3)	
24		$C_{24}H_{14}$(6,14)		$C_{24}H_{12}$(7,1)
26	$C_{26}H_{16}$(6,36)		$C_{26}H_{14}$(7,10)	
28		$C_{28}H_{16}$(7,68)		$C_{28}H_{14}$(8,9)
30	$C_{30}H_{18}$(7,118)		$C_{30}H_{16}$(8,67)	
32		$C_{32}H_{18}$(8,329)		$C_{32}H_{16}$(9,55)
34	$C_{34}H_{20}$(8,411)		$C_{34}H_{18}$(9,396)	
36		$C_{36}H_{20}$(9,1601)		
38	$C_{38}H_{22}$(8,1489)			
40				

[a] The first number in parentheses is the number of rings and the second is the number of isomers, including the diradical benzenoid isomers.

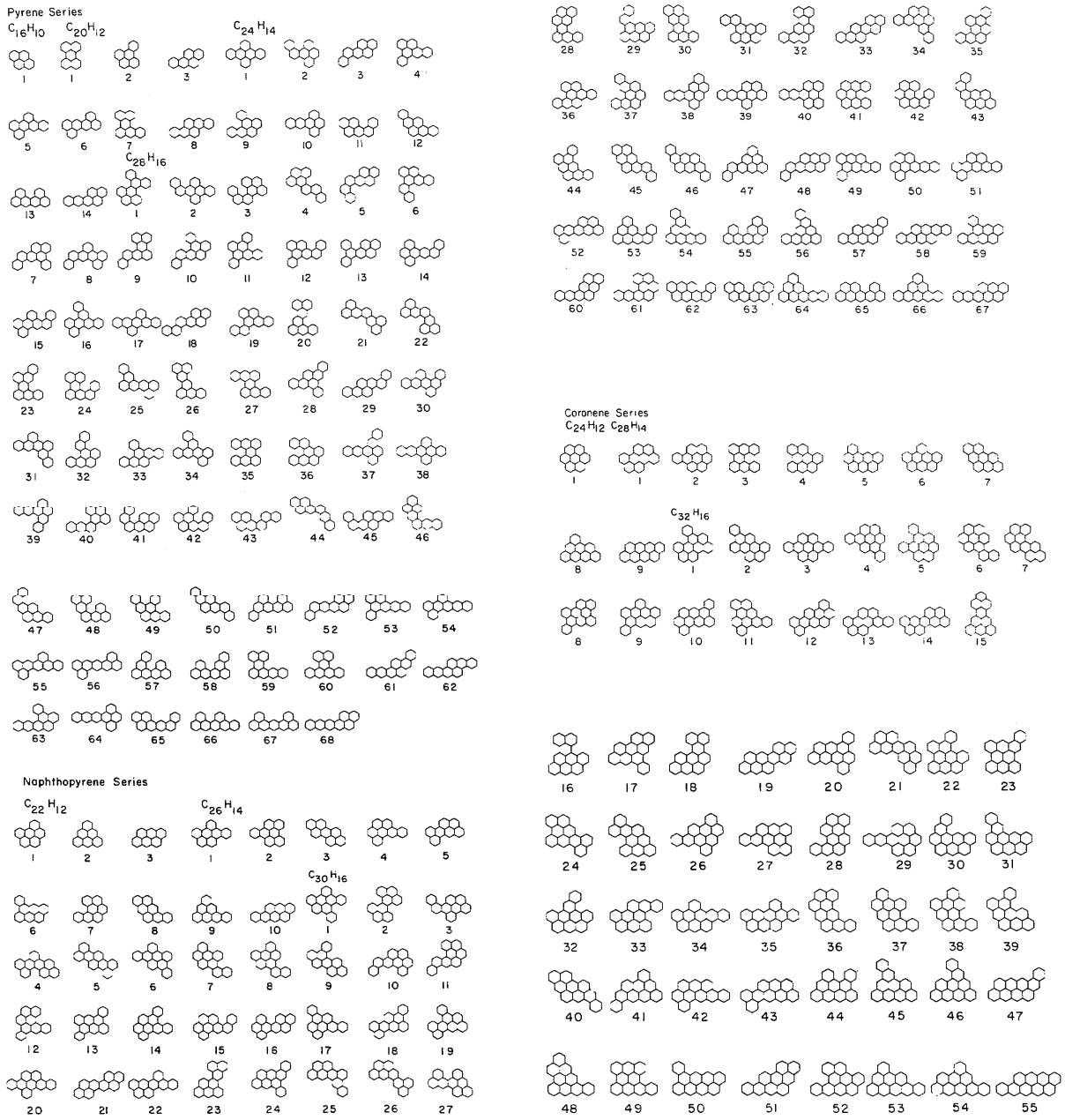

FIG 1. Structures of isomers in the pyrene, naphthopyrene, and coronene series.

2. Standard Thermodynamic Properties of Polycyclic Aromatic Isomer Groups

When isomers are in equilibrium, the standard Gibbs energy of formation $\Delta_f G^\circ(\mathrm{I})$ of the isomer groups is defined by [16,17]

$$\Delta_f G^\circ(\mathrm{I}) = -RT \ln \sum_{i=1}^{N_\mathrm{I}} \exp(-\Delta_f G_i^\circ/RT), \qquad (1)$$

where $\Delta_f G_i^\circ$ is the standard Gibbs energy of formation of an individual isomer and N_I is the number of isomers in an isomer group. The equilibrium mole fractions r_i of various isomers in a group can be calculated using

$$r_i = \frac{y_i}{y_\mathrm{I}} = \exp\{[\Delta_f G^\circ(\mathrm{I}) - \Delta_f G_i^\circ]/RT\}, \qquad (2)$$

where y_I is the sum of the mole fractions of the individual

TABLE 2. Numbers of isomers in thermodynamic tables

Formulas	Number of isomers	Number of diradicals	Number of helicenes	Number in tables
Pyrene series				
$C_{16}H_{10}$	1	0	0	1
$C_{20}H_{12}$	3	0	0	3
$C_{24}H_{14}$	14	1	0	13
$C_{28}H_{16}$	68	6	8	55[a]
Naphthopyrene series				
$C_{22}H_{12}$	3	1	0	2
$C_{26}H_{14}$	10	1	0	9
$C_{30}H_{16}$	87	9	2	76
Coronene series				
$C_{24}H_{12}$	1	0	0	1
$C_{28}H_{14}$	9	1	0	8
$C_{32}H_{16}$	55	9	0	46

[a] One diradical is a helicene.

isomers. The corresponding equations for the other standard thermodynamic properties $C_p^\circ(\mathrm{I})$, $S^\circ(\mathrm{I})$, and $\Delta_f H^\circ(\mathrm{I})$ can be derived by differentiating Eq. (1) with respect to temperature.[18] When standard Gibbs energies of formation of isomer groups are used in equilibrium calculations for ideal gases the equilibrium mole fractions of isomer groups are obtained.

For the polycyclic aromatic hydrocarbons the standard thermodynamic properties for an isomer group are interrelated by

$$\Delta_f G^\circ(\mathrm{I}) = \Delta_f H^\circ(\mathrm{I}) - T\left[S^\circ(\mathrm{I}) - n_C S^\circ_{\text{graphite}} - (n_H/2)S^\circ_{H_2}(g)\right], \quad (3)$$

where n_C is the number of carbon atoms and n_H is the number of hydrogen atoms.

3. Calculations of Standard Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons using the Benson Method

Experimental data on the polycyclic aromatic hydrocarbons are limited to the smaller molecules. Fortunately enough data were available for Stein, Golden, and Benson[19,20] to obtain group values for $C_B-(H)$, $C_{FR}-(C_{FR})(C_B)_2$, and $C_{FR}-(C_{FR})_2(C_B)$ groups; the group values of $C_{FR}-(C_{FR})_3$ were evaluated from graphite. The significance of these symbols is described in Benson's book.[19] The average difference between predicted and measured $\Delta_f H^\circ(298)$ for 11 polycyclic aromatic hydrocarbons was <2 kcal mol^{-1} and generally was within experimental uncertainties. More recently, Stein and Fahr[21] have provided Benson group values with C_p° values up to 3000 K. Although these values are similar to those of Stein, Golden, and Benson,[20] two major changes were made: (i) heat capacity values were calculated using the harmonic oscillator–rigid rotor approximation, and (ii) values of C_p° for the $[C_{FR}-(C_{FR})_3]$ group were derived from pyrene frequencies[22] rather than from graphite. These values are given in Table A.1 in the Appendix.

The procedures used in the estimation of chemical thermodynamic properties of the gaseous polycyclic aromatic hydrocarbons have been described in the preceding article.[1] The latest values have been used for various thermodynamic quantities.[23–25] Comparisons between properties of polycyclic aromatic hydrocarbons calculated using the Benson method and given in the TRC Thermodynamic Tables[26] for benzene, naphthalene, anthracene, and phenanthrene up to 1500 K were given in the preceding paper. There is a serious shortage of experimental data on polycyclic aromatic hydrocarbons. The only additional species for which a literature comparison is possible is pyrene. Pedley, Naylor, and Kirby[27] have selected the best value of the enthalpy of formation of pyrene gas at 298.15 K to be that determined by Smith *et al.*,[28] 225.7 ± 1.2 kJ mol^{-1}. The Benson method with the parameters we have used yields 230.5 kJ mol^{-1}. Since Smith *et al.*, studied vapor pressures over a range of temperatures and Wong and Westrum[29] obtained entropies of solid pyrene from low-temperature calorimetric studies, Smith *et al.*[28] were able to calculate chemical thermodynamic properties from 200 to 600 K. At the three temperatures at which their table overlaps ours, the average difference in C_p° is 2.6 J K^{-1} mol^{-1}, in S° is 0.9 J K^{-1} mol^{-1}, in $\Delta_f H^\circ$ is 5.0 kJ mol^{-1}, and in $\Delta_f G^\circ$ is 5.0 kJ mol^{-1}. These are all within the uncertainties that Benson states for his method, that is ± 4 J K^{-1} mol^{-1} for C_p° and S°, and ± 8 kJ mol^{-1} for $\Delta_f H^\circ$ and $\Delta_f G^\circ$.

All values of thermodynamic quantities in this article are for a standard state pressure of 1 bar (0.1 MPa) in accordance with the recommendation of the International Union of Pure and Applied Chemistry.[30]

4. Tables of Standard Thermodynamic Properties of Polycyclic Aromatic Isomer Groups in the Pyrene, Naphthopyrene, and Coronene Series

In Tables 3–8 all of the values have been estimated using the Benson method. Since the increments from one isomer group to the next are C_4H_2 in each series, the increments in the properties are given for each series at each temperature. These increments provide a basis for a linear extrapolation of standard thermodynamic properties to polycyclic aromatic isomer groups to higher carbon number.

Table 7 gives $H^\circ(\mathrm{I}, T)-H^\circ(\mathrm{I}, 298.15\ \mathrm{K})$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H^\circ(\mathrm{I}, T)-H^\circ(\mathrm{I}, 298.15\ \mathrm{K}) + \Delta_f H^\circ(\mathrm{I}, 298.15\ \mathrm{K})$, the standard enthalpy for the isomer group relative to the elements of 298.15 K. This quantity allows the direct calculation of heat effects when the reactants and products are at different temperatures.

5. Equilibrium Mole Fractions Within Polycyclic Aromatic Isomer Groups

The equilibrium mole fractions within isomer groups calculated from standard Gibbs energies of formation are given in Table 9 for the ideal gas state. Since the uncertainties in $\Delta_f G^\circ(\mathrm{I})$ and $\Delta_f G_i^\circ$ are about the same, the uncertainty in

Table 3. Standard heat capacity at constant pressure(J/K mol) for three series of polycyclic aromatic hydrocarbons

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10	204.8	206.0	333.5	418.5	491.6	551.7	581.6	598.8	609.7
C20H12	261.2	262.6	419.3	522.8	611.6	684.5	720.7	741.6	754.8
C24H14	350.7	353.0	537.0	632.5	730.0	814.7	857.1	881.7	897.1
C28H16	384.4	386.4	601.4	734.4	849.4	946.0	994.4	1022.3	1040.0
Naphthopyrene series									
C22H12	279.2	280.8	453.4	563.4	656.5	732.2	769.4	790.5	803.8
C26H14	334.4	336.3	548.4	678.3	781.2	865.1	907.3	931.6	946.9
C30H16	446.9	449.2	639.0	772.3	893.8	994.7	1044.5	1072.9	1090.7
Coronene series									
C24H12	290.5	292.4	480.0	598.8	698.7	778.8	817.4	839.1	852.5
C28H14	344.7	346.8	563.7	702.2	818.6	911.8	956.8	982.2	997.8
C32H16	396.6	399.0	664.4	825.7	947.5	1045.4	1094.6	1122.8	1140.4

Table 3a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20-C16	56.3	56.6	85.8	104.4	120.0	132.8	139.1	142.8	145.1
C24-C20	89.5	90.5	117.7	109.7	118.4	130.2	136.5	140.1	142.3
C28-C24	33.7	33.4	64.4	101.9	119.5	131.3	137.2	140.6	142.8
Naphthopyrene series									
C26-C22	55.2	55.5	95.0	115.0	124.7	132.9	137.9	141.1	143.1
C30-C26	112.5	112.8	90.5	94.0	112.6	129.6	137.2	141.3	143.7
Coronene series									
C28-C24	54.2	54.4	83.7	103.4	119.9	133.1	139.5	143.1	145.3
C32-C28	51.9	52.3	100.7	123.6	128.9	133.6	137.8	140.7	142.6

Table 4. Standard entropy for polycyclic aromatic hydrocarbon isomer groups in J/K mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10	402.2	403.5	539.6	666.4	829.3	1041.6	1204.9	1336.7	1446.9
C20H12	467.2	468.8	640.9	799.9	1002.9	1266.6	1469.0	1632.2	1768.7
C24H14	521.5	523.7	754.8	951.5	1195.0	1509.2	1750.0	1944.1	2106.3
C28H16	617.9	620.3	870.3	1095.3	1378.4	1743.6	2023.1	2248.3	2436.4
Naphthopyrene series									
C22H12	478.7	480.4	664.9	835.8	1053.8	1336.3	1552.5	1726.7	1872.1
C26H14	543.7	545.8	769.4	976.8	1238.0	1572.8	1828.0	2033.3	2204.6
C30H16	609.1	611.8	889.4	1127.0	1424.9	1809.1	2102.8	2339.2	2536.5
Coronene series									
C24H12	487.2	489.0	684.6	866.7	1098.9	1399.6	1629.5	1814.4	1968.7
C28H14	562.2	564.4	794.9	1008.5	1280.6	1632.7	1901.8	2118.2	2298.7
C32H16	632.1	634.5	903.2	1155.2	1472.7	1878.0	2186.2	2433.7	2640.1

Table 4a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20-C16	65.0	65.3	101.3	133.4	173.6	225.0	264.1	295.6	321.8
C24-C20	54.3	54.9	113.9	151.6	192.1	242.6	281.0	311.8	337.6
C28-C24	96.4	96.6	115.5	143.8	183.5	234.5	273.2	304.2	330.1
Naphthopyrene series									
C26-C22	65.0	65.4	104.5	140.9	184.1	236.5	275.5	306.7	332.6
C30-C26	65.3	66.0	119.9	150.2	187.0	236.3	274.8	305.8	331.8
Coronene series									
C28-C24	75.1	75.4	110.3	141.8	181.7	233.1	272.3	303.8	330.1
C32-C28	69.8	70.2	108.3	146.7	192.1	245.3	284.4	315.5	341.3

Table 5. Standard enthalpy of formation for polycyclic aromatic hydrocarbon isomer groups in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10	230.5	230.4	218.1	211.0	206.7	208.2	212.6	216.1	217.0
C20H12	280.2	280.0	266.8	259.7	256.0	259.6	266.4	271.9	274.0
C24H14	331.7	331.6	326.6	322.4	319.7	324.3	332.1	338.2	340.1
C28H16	401.4	401.2	388.8	382.7	380.3	386.6	396.0	402.9	405.0
Naphthopyrene series									
C22H12	301.7	301.6	289.2	282.9	280.0	283.9	290.3	294.7	295.0
C26H14	351.2	351.0	338.5	334.3	334.4	341.4	349.9	355.4	356.1
C30H16	405.4	405.3	398.3	392.9	390.8	397.6	407.2	413.9	415.0
Coronene series									
C24H12	322.7	322.5	309.4	302.7	299.4	302.8	308.4	311.4	309.7
C28H14	372.2	372.0	357.5	350.4	347.6	353.3	361.4	366.5	366.2
C32H16	417.0	416.8	402.4	399.0	401.1	410.9	421.2	427.3	427.1

Table 5a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20-C16	49.6	49.6	48.8	48.7	49.3	51.5	53.9	55.8	57.0
C24-C20	51.6	51.6	59.7	62.8	63.6	64.6	65.7	66.3	66.1
C28-C24	69.6	69.6	62.2	60.2	60.6	62.3	63.8	64.7	64.8
Naphthopyrene series									
C26-C22	49.5	49.4	49.4	51.4	54.4	57.5	59.6	60.8	61.1
C30-C26	54.2	54.3	59.8	58.6	56.4	56.2	57.3	58.4	58.9
Coronene series									
C28-C24	49.5	49.4	48.1	47.7	48.2	50.5	53.0	55.1	56.5
C32-C28	44.8	44.8	44.9	48.6	53.5	57.6	59.8	60.8	60.9

Table 6. Standard Gibbs energy of formation for polycyclic aromatic hydrocarbon isomer groups

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10	332.8	333.4	405.9	482.5	599.8	796.3	991.7	1187.3	1379.9
C20H12	408.9	409.7	500.2	595.0	739.6	980.9	1220.3	1459.6	1695.1
C24H14	490.0	491.0	599.1	708.9	875.2	1152.3	1427.1	1701.8	1972.2
C28H16	576.8	577.9	699.7	825.4	1015.9	1333.0	1647.2	1961.2	2270.2
Naphthopyrene series									
C22H12	430.2	431.0	521.5	616.0	760.1	1000.3	1238.7	1477.1	1712.0
C26H14	506.3	507.3	615.5	727.2	895.8	1175.2	1451.8	1728.3	2000.6
C30H16	586.8	587.9	711.6	838.0	1029.3	1347.4	1662.6	1977.6	2287.7
Coronene series									
C24H12	452.3	453.1	544.2	639.5	784.7	1026.9	1267.5	1508.3	1746.0
C28H14	525.2	526.1	633.4	745.3	915.3	1198.2	1478.7	1759.1	2035.5
C32H16	595.0	596.1	720.4	848.4	1040.8	1358.6	1672.9	1987.0	2296.5

Table 6a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20-C16	76.1	76.2	94.3	112.5	139.8	184.6	228.6	272.3	315.2
C24-C20	81.1	81.3	98.9	113.9	135.6	171.4	206.8	242.2	277.1
C28-C24	86.8	86.9	100.6	116.5	140.7	180.7	220.1	259.4	298.0
Naphthopyrene series									
C26-C22	76.1	76.2	94.0	111.2	135.7	174.8	213.1	251.2	288.6
C30-C26	80.5	80.7	96.1	110.7	133.6	172.3	210.8	249.3	287.1
Coronene series									
C28-C24	72.9	73.1	89.2	105.7	130.5	171.3	211.2	250.8	289.6
C32-C28	69.8	69.9	86.9	103.1	125.5	160.4	194.3	227.9	261.0

Table 7. Standard enthalpy for polycyclic aromatic hydrocarbon isomer groups relative to isomer groups at 298.15 K in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10	.0	.4	54.8	130.7	268.3	531.1	815.4	1110.6	1413.0
C20H12	.0	.5	69.2	164.3	335.8	662.3	1014.7	1380.5	1754.8
C24H14	.0	.7	92.8	210.1	415.8	804.6	1223.9	1658.9	2103.8
C28H16	.0	.7	100.7	235.4	474.7	926.6	1413.2	1917.6	2433.5
Naphthopyrene series									
C22H12	.0	.5	74.8	177.4	361.8	711.5	1088.1	1478.3	1877.1
C26H14	.0	.6	90.0	214.0	434.6	848.9	1293.3	1753.3	2223.2
C30H16	.0	.8	110.9	252.9	504.7	980.1	1491.5	2021.1	2562.3
Coronene series									
C24H12	.0	.5	78.7	187.6	383.9	756.0	1156.2	1570.6	1993.7
C28H14	.0	.6	92.7	220.5	450.5	886.3	1354.9	1839.9	2335.2
C32H16	.0	.7	108.2	258.9	527.0	1028.4	1565.0	2119.6	2685.7

Table 7a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20-C16	.0	.1	14.5	33.6	67.5	131.1	199.3	269.8	341.8
C24-C20	.0	.2	23.5	45.8	79.9	142.4	209.2	278.4	349.0
C28-C24	.0	.1	7.9	25.2	58.9	122.0	189.3	258.8	329.7
Naphthopyrene series									
C26-C22	.0	.1	15.2	36.6	72.8	137.3	205.2	275.0	346.0
C30-C26	.0	.2	20.9	39.0	70.1	131.2	198.2	267.8	339.1
Coronene series									
C28-C24	.0	.1	14.0	32.8	66.6	130.3	198.6	269.3	341.5
C32-C28	.0	.1	15.5	38.4	76.6	142.1	210.1	279.7	350.6

Table 8. Standard enthalpy for polycyclic aromatic hydrocarbon isomer groups relative to the elements at 298.15 K in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10	230.5	230.9	285.3	361.2	498.8	761.7	1045.9	1341.2	1643.5
C20H12	280.2	280.7	349.4	444.5	616.0	942.4	1294.8	1660.6	2035.0
C24H14	331.7	332.4	424.5	541.9	747.5	1136.4	1555.6	1990.6	2435.6
C28H16	401.4	402.1	502.0	636.7	876.0	1328.0	1814.5	2319.0	2834.9
Naphthopyrene series									
C22H12	301.7	302.2	376.5	479.1	663.6	1013.3	1389.8	1780.0	2178.8
C26H14	351.2	351.8	441.2	565.2	785.8	1200.1	1644.5	2104.4	2574.3
C30H16	405.4	406.2	516.4	658.3	910.1	1385.5	1896.9	2426.5	2967.7
Coronene series									
C24H12	322.7	323.2	401.4	510.3	706.6	1078.7	1478.9	1893.3	2316.4
C28H14	372.2	372.8	464.9	592.6	822.6	1258.4	1727.1	2212.1	2707.4
C32H16	417.0	417.7	525.2	675.9	944.0	1445.4	1981.9	2536.6	3102.7

Table 8a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20-C16	49.6	49.8	64.1	83.3	117.2	180.8	248.9	319.5	391.5
C24-C20	51.6	51.7	75.1	97.4	131.5	193.9	260.8	330.0	400.6
C28-C24	69.6	69.7	77.5	94.8	128.5	191.6	258.9	328.4	399.3
Naphthopyrene series									
C26-C22	49.5	49.6	64.7	86.1	122.2	186.8	254.7	324.4	395.5
C30-C26	54.2	54.4	75.2	93.2	124.3	185.5	252.4	322.1	393.4
Coronene series									
C28-C24	49.5	49.6	63.4	82.3	116.1	179.8	248.1	318.8	390.9
C32-C28	44.8	44.9	60.3	83.2	121.4	186.9	254.9	324.5	395.3

Table 9. Equilibrium mole fractions within polycyclic aromatic hydrocarbon isomer groups

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C20H12									
1. perylene	.3228	.3226	.2910	.2616	.2314	.2036	.1887	.1796	.1734
2. benzo(e)pyrene	.6457	.6452	.5819	.5232	.4627	.4072	.3774	.3591	.3469
3. benzo(a)pyrene	.0315	.0322	.1271	.2152	.3059	.3893	.4339	.4613	.4797
C24H14									
1. dibenzo(fg,op)naphthacene	.7956	.7906	.2548	.0854	.0319	.0142	.0095	.0075	.0064
2. naphtho(8,1,2-ghi)chrysene	.0137	.0144	.1520	.2225	.2473	.2512	.2489	.2462	.2438
3. benzo(pqr)picene	.0019	.0020	.0122	.0145	.0139	.0129	.0125	.0123	.0123
4. dibenzo(a,e)pyrene	.0777	.0790	.1113	.0703	.0421	.0271	.0217	.0192	.0178
5. benzo(b)perylene	.0777	.0790	.1113	.0703	.0421	.0271	.0217	.0192	.0178
6. zethrene	.0019	.0020	.0122	.0145	.0139	.0129	.0125	.0123	.0123
7. benzo(a)perylene	.0137	.0144	.1520	.2225	.2473	.2512	.2489	.2462	.2438
8. dibenzo(b,def)chrysene	.0019	.0020	.0122	.0145	.0139	.0129	.0125	.0123	.0123
9. dibenzo(def,p)chrysene	.0137	.0144	.1520	.2225	.2473	.2512	.2489	.2462	.2438
10. dibenzo(de,qr)naphthacene	.0009	.0010	.0061	.0072	.0070	.0065	.0062	.0062	.0062
11. dibenzo(c,mno)chrysene	.0003	.0004	.0166	.0458	.0817	.1201	.1431	.1581	.1686
12. benzo(rst)pentaphene	.0009	.0010	.0061	.0072	.0070	.0065	.0062	.0062	.0062
14. naphtho(2,1,8-qra)naphthacene	.0000	.0000	.0013	.0030	.0046	.0062	.0072	.0079	.0085
C28H16									
1. tribenzo(f,ij,no)tetraphene	.0288	.0297	.1348	.1769	.1790	.1619	.1488	.1399	.1334
2. tribenzo(a,fg,op)tetracene	.3258	.3252	.1975	.1118	.0610	.0349	.0260	.0218	.0195
4. naphtho(2,1,8-def)picene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
5. dibenzo(a,pqr)picene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
6. benzo(a)naphtho(8,1,2-fgh)tetracene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
7. naphtho(1,2,3,4-bqr)picene	.0450	.0445	.0158	.0073	.0034	.0018	.0013	.0011	.0010
8. naphtho(1,2-b)perylene	.0450	.0445	.0158	.0073	.0034	.0018	.0013	.0011	.0010
9. naphtho(2,1-a)perylene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
10. dibenzo(j,pqr)picene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
11. benzo(fg)naphtho(3,2,1-op)tetracene	.3258	.3252	.1975	.1118	.0610	.0349	.0260	.0218	.0195
12. tribenzo(f,m,pqr)tetraphene	.0080	.0031	.0216	.0230	.0202	.0167	.0149	.0140	.0135
13. dibenzo(f,pqr)picene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
14. tribenzo(a,hi,mn)tetracene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
15. naphtho(1,2-e)perylene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
16. dibenzo(a,e)perylene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
17. dibenzo(fg,qr)pentacene	.0450	.0445	.0158	.0073	.0034	.0018	.0013	.0011	.0010
18. naphtho(8,1,2-cde)picene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
19. benzo(c)naphtho(8,1,2-ghi)tetraphene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
20. benzo(a)zethrene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
21. dibenzo(de,kl)pentaphene	.0005	.0006	.0009	.0007	.0006	.0004	.0004	.0004	.0003
23. dibenzo(a,n)perylene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
25. dibenzo(de,ij)pentaphene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
26. benzo(f)zethrene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
27. dibenzo(a,j)perylene	.0014	.0015	.0295	.0728	.1183	.1548	.1711	.1797	.1845
28. dibenzo(h,rst)pentaphene	.0225	.0223	.0079	.0036	.0017	.0009	.0007	.0005	.0005
29. dibenzo(b,tuv)picene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
30. dibenzo(b,j)perylene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135
31. dibenzo(fg,ij)pentaphene	.0225	.0223	.0079	.0036	.0017	.0009	.0007	.0005	.0005
32. phrenthro(1,2,3,4-pqr)tetracene	.0014	.0015	.0295	.0728	.1183	.1548	.1711	.1797	.1845
33. benzo(c)naphtho(1,2,3,4-pqr)tetracene	.0080	.0081	.0216	.0230	.0202	.0167	.0149	.0140	.0135

Table 9. Equilibrium mole fractions within polycyclic aromatic hydrocarbon isomer groups -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
34. dibenzo(b,c)perylene	.0040	.0041	.0108	.0115	.0101	.0083	.0075	.0070	.0067
37. naphtho(2,1,3-fgh)pentacene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
38. dibenzo(fg,st)pentaphene	.0225	.0223	.0079	.0036	.0017	.0009	.0007	.0005	.0005
39. benzo(de)naphtho(1,2,3-qr)tetracene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
40. dibenzo(de,uv)pentaphene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
43. benzo(c)naphthol(8,1,2-mno)tetraphene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
44. naphtho(8,1,2-cde)pentaphene	.0000	.0000	.0002	.0003	.0004	.0004	.0004	.0005	.0005
45. tribenzo(c,m,pqr)tetraphene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
46. naphtho(8,1,2-opq)pentacene	.0000	.0000	.0003	.0010	.0022	.0038	.0049	.0058	.0064
47. dibenzo(o,rst)pentaphene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
49. naphtho(1,2,3,4-rst)pentaphene	.0007	.0007	.0147	.0364	.0592	.0774	.0856	.0898	.0923
50. dibenzo(c,rst)pentaphene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
52. benzo(a)naphtho(2,1,8-hij)tetracene	.0000	.0000	.0002	.0003	.0004	.0004	.0004	.0005	.0005
53. benzo(a)naphtho(8,1,2-cde)tetracene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
54. dibenzo(de,st)pentacene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
55. dibenzo(de,qr)pentacene	.0011	.0011	.0017	.0015	.0011	.0009	.0007	.0007	.0007
56. heptazethrene	.0000	.0000	.0002	.0003	.0004	.0004	.0004	.0005	.0005
59. naphtho(2,3-a)perylene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
60. dibenzo(a,f)perylene	.0007	.0007	.0147	.0364	.0592	.0774	.0856	.0898	.0923
61. benzo(vwx)hexaphene	.0000	.0000	.0002	.0003	.0004	.0004	.0004	.0005	.0005
62. anthra 2,1,9-qra)tetracene	.0000	.0000	.0002	.0003	.0004	.0004	.0004	.0005	.0005
63. phenanthro(9,10,1-hif)tetracene	.0002	.0002	.0024	.0047	.0067	.0080	.0086	.0090	.0093
64. dibenzo(de,uv)pentacene	.0000	.0000	.0001	.0002	.0002	.0002	.0002	.0002	.0002
65. benzo(a)naphtho(8,1,2-lmn)tetracene	.0000	.0000	.0002	.0003	.0004	.0004	.0004	.0005	.0005
68. naphtho(2,1,8-jkl)pentacene	.0000	.0000	.0000	.0001	.0001	.0002	.0002	.0003	.0003
Naphthopyrene series									
C22H12									
1. benzo(ghi)perylene	.9535	.9524	.8207	.7086	.6020	.5112	.4652	.4377	.4197
3. dibenzo(def,mno)chrysene	.0465	.0476	.1793	.2914	.3980	.4888	.5348	.5623	.5803
C26H14									
1. dibenzo(e,ghi)perylene	.6310	.6301	.4931	.3444	.2113	.1258	.0942	.0791	.0706
2. naphtho(1,2,3,4-ghi)perylene	.3155	.3151	.2465	.1722	.1057	.0629	.0471	.0395	.0353
3. dibenzo(cd,lm)perylene	.0038	.0039	.0135	.0177	.0175	.0150	.0135	.0127	.0122
4. dibenzo(b,ghi)perylene	.0154	.0157	.0539	.0708	.0698	.0601	.0542	.0508	.0488
5. naphtho(8,1,2-bcd)perylene	.0154	.0157	.0539	.0708	.0698	.0601	.0542	.0508	.0488
6. benzo(e)anthanthrene	.0154	.0157	.0539	.0708	.0698	.0601	.0542	.0508	.0488
7. dibenzo(a,ghi)perylene	.0027	.0029	.0735	.2242	.4098	.5583	.6204	.6511	.6678
8. benzo(a)anthanthrene	.0004	.0004	.0059	.0146	.0231	.0288	.0311	.0326	.0338
10. benzo(b)anthanthrene	.0004	.0004	.0059	.0146	.0231	.0288	.0311	.0326	.0338
C30H16									
1. benzo(e)naphtho(1,2,3,4-ghi)perylene	.2102	.2140	.3002	.2084	.1347	.0881	.0696	.0600	.0542
2. tetrabenzo(de,hi,mn,qr)tetracene	.0002	.0002	.0112	.0339	.0653	.0978	.1145	.1234	.1281
3. benzo(ghi)naphtho(1,2-e)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
4. benzo(lm)naphtho(1,8-ab)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
5. terrylene	.0073	.0073	.0060	.0034	.0019	.0011	.0009	.0008	.0007
6. tribenzo(fg,ij,rst)pentaphene	.5948	.5867	.1099	.0329	.0115	.0047	.0030	.0023	.0020
7. benzo(ghi)naphtho(2,1-e)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
8. phenanthro(1,2,3,4-ghi)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
9. benzo(a)peropyrene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
10. benzo(ghi)naphtho(1,2-b)perylene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
11. benzo(ghi)naphtho(2,1-a)perylene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
12. tribenzo(a,e,ghi)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
13. dibenzo(e,h)anthanthrene	.0290	.0293	.0240	.0135	.0076	.0045	.0035	.0030	.0027

Table 9. Equilibrium mole fractions within polycyclic aromatic hydrocarbon isomer groups -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
14. tribenzo(b,e,ghi)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
15. benzo(ghi)naphtho(2,1-b)perylene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
16. benzo(pqr)naphtho(2,1,8-def)picene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
17. benzo(rst)naphtho(2,1,8-fgh)pentaphene	.0290	.0293	.0240	.0135	.0076	.0045	.0035	.0030	.0027
18. tribenzo(de,ij,rst)pentaphene	.0290	.0293	.0240	.0135	.0076	.0045	.0035	.0030	.0027
19. benzo(a)naphtho(2,1,8-cde)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
20. benzo(qr)naphtho(2,1,8,7-fghi)pentacene	.0290	.0293	.0240	.0135	.0076	.0045	.0035	.0030	.0027
21. benzo(pq)naphtho(8,1,2-cde)picene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
22. benzo(qr)naphtho(2,1,8,7-defg)pentacene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
23. naphtho(8,1,2-fgh)zethrene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
24. dibenzo(a,e)anthanthrene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
25. benzo(ij)naphtho(2,1,8,7-defg)pentaphene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
26. benzo(de)naphtho(2,1,8,7-ijkl)pentaphene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
28. benzo(a)naphtho(2,1,8-lmn)perylene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
29. naphtho(2,1-e)anthanthrene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
30. benzo(a)naphtho(8,1,2-klm)perylene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
31. naphtho(1,2-e)anthanthrene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
32. anthra(9,1,2-bcd)perylene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
33. benzo(g,hi)naphtho(8,1,2-cde)picene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
34. phenanthro(3,4,5,6-fghij)pentaphene	.0004	.0004	.0013	.0014	.0013	.0011	.0010	.0010	.0009
35. tribenzo(a,ghi,k)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
36. benzo(a)naphtho(1,2,3,4-ghi)perylene	.0051	.0053	.0328	.0429	.0445	.0421	.0400	.0385	.0375
37. tribenzo(a,ghi,k)perylene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
38. naphtho(2,3-e)anthanthrene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
39. benzo(st)naphtho(2,1,8,7-defg)pentacene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
40. anthra(1,2,3,4-ghi)perylene	.0004	.0004	.0013	.0014	.0013	.0011	.0010	.0010	.0009
43. naphtho(1,2-a)anthanthrene	.0000	.0000	.0004	.0018	.0049	.0096	.0132	.0159	.0179
44. dibenzo(a,n)anthanthrene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
45. naphtho(2,1-a)anthanthrene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
46. pyranthrene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
48. naphtho(1,2-b)anthanthrene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
49. dibenzo(b,r)anthanthrene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
50. benzo(uv)naphtho(2,1,8,7-defg)pentacene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
51. benzo(de)naphtho(2,1,8,7-qrst)pentacene	.0007	.0007	.0026	.0028	.0025	.0022	.0020	.0019	.0019
52. benzo(de)naphtho(2,1,8,7-opqr)pentacene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
57. dibenzo(a,k)anthanthrene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
58. dibenzo(b,k)anthanthrene	.0000	.0000	.0003	.0006	.0008	.0010	.0012	.0012	.0013
59. dibenzo(b,e)anthanthrene	.0001	.0001	.0036	.0088	.0147	.0201	.0230	.0247	.0259
60. naphtho(2,3-a)anthanthrene	.0037	.0038	.0268	.0371	.0402	.0394	.0380	.0370	.0362
61. benzo(uv)naphtho(2,1,8-defg)pentaphene	.0037	.0038	.0268	.0371	.0402	.0394	.0380	.0370	.0362
62. naphtho(2,1-b)anthanthrene	.0037	.0038	.0268	.0371	.0402	.0394	.0380	.0370	.0362
63. dinaphtho(8,1,2-cde:2′,1′,8′-hij)naphthacene	.0000	.0000	.0002	.0009	.0024	.0048	.0066	.0079	.0090
67. naphtho(2,3-b)anthanthrene	.0000	.0000	.0000	.0001	.0003	.0005	.0007	.0008	.0009
Coronene series									
C28H14									
1. dibenzo(hi,qr)anthanthrene	.3042	.3041	.2919	.2777	.2594	.2383	.2251	.2162	.2099
2. benzo(a)coronene	.1521	.1521	.1460	.1389	.1297	.1192	.1125	.1081	.1049
3. phenanthro(1,10,9,8-opqra)perylene	.0761	.0760	.0730	.0694	.0649	.0596	.0563	.0540	.0525
4. naphtho(8,1,2-efg)anthanthrene	.3042	.3041	.2919	.2777	.2594	.2383	.2251	.2162	.2099
5. dibenzo(cd,hi)anthanthrene	.0074	.0076	.0319	.0571	.0857	.1139	.1294	.1388	.1451
6. dibenzo(cd,fg)anthanthrene	.1521	.1521	.1460	.1389	.1297	.1192	.1125	.1081	.1049
7. naphtho(2,1,8-hij)anthanthrene	.0037	.0038	.0159	.0286	.0429	.0570	.0647	.0694	.0725
9. dibenzo(cd,lm)anthanthrene	.0002	.0002	.0035	.0117	.0283	.0545	.0744	.0892	.1003
C32H16									

Table 9. Equilibrium mole fractions within polycyclic aromatic hydrocarbon isomer groups -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
1. tribenzo(e,hi,qr)anthanthrene	.0016	.0017	.0232	.0535	.0736	.0759	.0725	.0694	.0669
2. tribenzo(b,hi,qr)anthanthrene	.0090	.0091	.0170	.0169	.0125	.0082	.0063	.0054	.0049
3. dibenzo(a,j)coronene	.0023	.0023	.0042	.0042	.0031	.0020	.0016	.0014	.0012
4. dibenzo(a,g)coronene	.0045	.0046	.0085	.0085	.0063	.0041	.0032	.0027	.0024
5. dibenzo(a,d)coronene	.9571	.9563	.7934	.5478	.3046	.1553	.1043	.0808	.0677
6. naphtho(1,2-a)coronene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
7. naphtho(8,1,2-abc)peropyrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
8. tribenzo(b,fg,qr)anthanthrene	.0090	.0091	.0170	.0169	.0125	.0082	.0063	.0054	.0049
9. tribenzo(a,cd,fg)anthanthrene	.0090	.0091	.0170	.0169	.0125	.0082	.0063	.0054	.0049
10. tribenzo(a,cd,hi)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
11. benzo(a)naphtho(8,1,2-efg)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
12. benzo(ghi)terrylene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
13. benzo(qr)naphtho(3,2,1-hi)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
14. dibenzo(bc,mn)peropyrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
16. dinaphtho(1,8-ab:8′,1′,2′,3′-fghi)perylene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
17. naphtho(1,2,3,4-ijk)peropyrene	.0001	.0001	.0009	.0017	.0021	.0020	.0018	.0017	.0017
18. dibenzo(ghi,lm)naphtho(1,8-ab)perylene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
19. naphtho(2,1,8-bcd)peropyrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
20. benzo(a)naphtho(2,1,8-cde)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
21. dibenzo(bc,qr)peropyrene	.0000	.0000	.0001	.0004	.0007	.0009	.0010	.0011	.0012
22. tribenzo(e,hi,op)anthanthrene	.0016	.0017	.0232	.0535	.0736	.0759	.0725	.0694	.0669
23. tribenzo(b,fg,op)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
24. benzo(fg)naphtho(1,8-ab)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
26. tribenzo(b,hi,op)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
27. benzo(b)naphtho(8,1,2-nop)anthanthrene	.0002	.0002	.0019	.0035	.0041	.0039	.0036	.0035	.0034
28. benzo(hi)naphtho(1,2,3-qr)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
29. naphtho(2,3-a)coronene	.0000	.0000	.0001	.0004	.0007	.0009	.0010	.0011	.0012
30. benzo(cd)naphtho(1,2,3-hi)anthanthrene	.0000	.0000	.0003	.0023	.0080	.0173	.0240	.0286	.0320
31. benzo(cd)naphtho(3,2,1-hi)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
32. benzo(cd)naphtho(3,2,1-fg)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
33. tribenzo(a,hi,op)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
34. tribenzo(cd,fg,k)anthanthrene	.0016	.0017	.0232	.0535	.0736	.0759	.0725	.0694	.0669
35. tribenzo(cd,hi,k)anthanthrene	.0016	.0017	.0232	.0535	.0736	.0759	.0725	.0694	.0669
36. benzo(a)naphtho(2,1,8-lmn)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
37. tribenzo(cd,fg,j)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
38. benzo(a)naphtho(8,1,2-nop)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
39. benzo(e)naphtho(2,1,8-hij)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
40. benzo(a)naphtho(2,1,8-hij)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
42. benzo(b)naphtho(2,1,8-lmn)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
43. benzo(lm)naphtho(1,8-ab)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
47. benzo(a)naphtho(8,1,2-klm)anthanthrene	.0000	.0000	.0000	.0001	.0005	.0009	.0012	.0014	.0016
49. tribenzo(a,fg,op)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
50. benzo(n)naphtho(8,1,2-bcd)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
51. benzo(b)naphtho(2,1,8-hij)anthanthrene	.0000	.0000	.0002	.0007	.0014	.0019	.0021	.0022	.0023
52. benzo(b)naphtho(8,1,2-efg)anthanthrene	.0000	.0000	.0025	.0110	.0243	.0363	.0417	.0446	.0463
55. benzo(b)naphtho(8,1,2-klm)anthanthrene	.0000	.0000	.0000	.0001	.0005	.0009	.0012	.0014	.0016

the difference is nearly independent of the relative values of the two parameters, but the absolute uncertainty does increase with temperature.

The substances in the tables are named according to Dias,[6] who follows the IUPAC Revised and Collected Recommendations for the Nomenclature of Organic Chemistry, 1978.[31]

Table 9 shows that there are significant changes in the distribution of isomers within an isomer group when the temperature is changed from 298 K to 3000 K. At higher temperatures, the relative stabilities are determined primarily by the entropy. The distribution becomes more uniform as the temperature is raised.

6. Standard Thermodynamic Properties of Individual Polycyclic Aromatic Hydrocarbons

The values of C_p°, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ calculated using the Benson method for the polycyclic aromatic hydrocarbons are given in Tables 10 to 13 in joules for a standard state pressure of 1 bar.

7. Discussion

The increments in the standard Gibbs energy of formation for the pyrene isomer groups per C_4H_2 are very close to those for the benzene series.[1] The increments for the naphthopyrene series are a little smaller, and those for the coronene series are still smaller. However, Fig. 2 of the preceding article[1] provides a useful guide to the partial pressures of acetylene and hydrogen that will cause higher isomer groups to predominate at a given temperature.

It is interesting to observe that the zethrenes (number 6 of $C_{24}H_{14}$, numbers 20 and 26 of $C_{28}H_{16}$) do not contribute significantly to the isomer group thermodynamic properties. These molecules are remarkable because two double bonds in the center of the molecules are fixed. For this reason we were not sure that they should be included in the current calculations. However, this bond fixation appears to have no influence on the aromatic character of the absorption spectra and the reactivity.[32]

In making equilibrium calculations on polycyclic aromatic hydrocarbons in flames it is convenient to use isomer groups because of the geometric increase in the number of isomers with carbon numbers. It is also convenient to deal with series, such as the three described here, because the standard thermodynamic properties are very nearly a linear function of the number of C_4H_2 increments added to the leading member of the series. When one or more reactants are available to a system at a constant chemical potential, their terms can be removed from the fundamental equation of thermodynamics by use of a Legendre transform to obtain a new thermodynamic potential that is a minimum at equilibrium.[33] Thus a new thermodynamic potential for isomer groups of polycyclic aromatic hydrocarbons can be defined at specified chemical potentials of acetylene and hydrogen. This makes it possible to treat a series as a single species in an equilibrium calculation.

Table 10. Standard heat capacity at constant pressure for polycyclic aromatic hydrocarbons in J/K mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10									
pyrene	204.8	206.0	333.5	418.5	491.6	551.7	581.6	598.8	609.7
C20H12									
1. perylene	257.7	259.0	414.8	519.3	609.4	683.4	720.1	741.2	754.6
2. benzo(e)pyrene	257.7	259.0	414.8	519.3	609.4	683.4	720.1	741.2	754.6
3. benzo(a)pyrene	257.7	259.0	414.8	519.3	609.4	683.4	720.1	741.2	754.6
C24H14									
1. dibenzo(fg,op)raphthacene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
2. naphtho(8,1,2-ghi)chrysene	306.1	307.8	494.8	619.1	725.9	813.2	856.3	881.0	896.6
3. benzo(pqr)picere	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
4. dibenzo(a,e)pyrene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
5. benzo(b)perylere	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
6. zethrene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
7. benzo(a)perylere	306.1	307.8	494.8	619.1	725.9	813.2	856.3	881.0	896.6
8. dibenzo(b,def)chrysene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
9. dibenzo(def,p)chrysene	306.1	307.8	494.8	619.1	725.9	813.2	856.3	881.0	896.6
10. dibenzo(de,qr)naphthacene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
11. dibenzo(c,mno)chrysene	306.1	307.8	494.8	619.1	725.9	813.2	856.3	881.0	896.6
12. benzo(rst)pentaphene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
14. naphtho(2,1,8-qra)naphthacene	310.5	312.1	496.0	620.2	727.2	815.1	858.6	883.6	899.4
C28H16									
1. tribenzo(f,ij,no)tetraphene	354.5	356.5	574.8	718.9	842.3	943.0	992.5	1020.9	1038.7
2. tribenzo(a,fg,op)tetracene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
4. naphtho(2,1,8-def)picene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
5. dibenzo(a,pqr)picene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
6. benzo(a)naphtho(8,1,2-fgh)tetracene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
7. naphtho(1,2,3,4-bqr)picene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
8. naphtho(1,2-b)perylene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
9. naphtho(2,1-a)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
10. dibenzo(j,pqr)picene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
11. benzo(fg)naphtho(3,2,1-op)tetracene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
12. tribenzo(f,m,pqr)tetraphene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
13. dibenzo(f,pqr)picene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
14. tribenzo(a,hi,mn)tetracene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
15. naphtho(1,2-e)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
16. dibenzo(a,e)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
17. dibenzo(fg,qr)pentacene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
18. naphtho(8,1,2-cde)picene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
19. benzo(c)naphtho(8,1,2-ghi)tetraphene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
20. benzo(a)zethrene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
21. dibenzo(de,kl)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
23. dibenzo(a,n)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
25. dibenzo(de,ij)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
26. benzo(f)zethrene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
27. dibenzo(a,j)perylene	354.5	356.5	574.8	718.9	842.3	943.0	992.5	1020.9	1038.7
28. dibenzo(h,rst)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
29. dibenzo(b,tuv)picene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2

Table 10. Standard heat capacity at constant pressure for polycyclic aromatic hydrocarbons in J/K mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
30. dibenzo(b,j)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
31. dibenzo(fg,ij)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
32. phrenthro(1,2,3,4-pqr)tetracene	354.5	356.5	574.8	718.9	842.3	943.0	992.5	1020.9	1038.7
33. benzo(c)naphtho(1,2,3,4-pqr)tetracene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
34. dibenzo(b,c)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
37. naphtho(2,1,8-fgh)pentacene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
38. dibenzo(fg,st)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
39. benzo(de)naphtho(1,2,3-qr)tetracene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
40. dibenzo(de,uv)pentaphene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
43. benzo(c)naphthol(8,1,2-mno)tetraphene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
44. naphtho(8,1,2-cde)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
45. tribenzo(c,m,pqr)tetraphene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
46. naphtho(8,1,2-cpq)pentacene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
47. dibenzo(o,rst)pentaphene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
49. naphtho(1,2,3,4-rst)pentaphene	354.5	356.5	574.8	718.9	842.3	943.0	992.5	1020.9	1038.7
50. dibenzo(c,rst)pentaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
52. benzo(a)naphtho(2,1,8-hij)tetracene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
53. benzo(a)naphtho(8,1,2-cde)tetracene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
54. dibenzo(de,st)pentacene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
55. dibenzo(de,qr)pentacene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
56. heptazethrene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
59. naphtho(2,3-a)perylene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
60. dibenzo(a,f)perylene	354.5	356.5	574.8	718.9	842.3	943.0	992.5	1020.9	1038.7
61. benzo(vwx)hexaphene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
62. anthra 2,1,9-qra)tetracene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
63. phenanthro(9,10,1-hif)tetracene	358.9	360.8	576.1	720.0	843.7	944.9	994.8	1023.4	1041.5
64. dibenzo(de,uv)pentacene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
65. benzo(a)naphtho(8,1,2-lmn)tetracene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
68. naphtho(2,1,8-jkl)pentacene	363.3	365.1	577.3	721.0	845.0	946.8	997.1	1026.0	1044.2
Naphthopyrene series									
C22H12									
1. benzo(ghi)perylene	274.11	275.70	447.41	559.07	654.05	731.08	768.73	790.14	803.52
3. dibenzo(def,mno)chrysene	274.11	275.70	447.41	559.07	654.05	731.08	768.73	790.14	803.52
C26H14									
1. dibenzo(e,ghi)perylene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
2. naphtho(1,2,3,4-ghi)perylene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
3. dibenzo(cd,lm)perylene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
4. dibenzo(b,ghi)perylene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
5. naphtho(8,1,2-bcd)perylene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
6. benzo(e)anthanthrene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
7. dibenzo(a,ghi)perylene	322.5	324.4	527.4	658.9	770.5	860.9	905.0	930.0	945.6
8. benzo(a)anthanthrene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
10. benzo(b)anthanthrene	326.9	328.8	528.7	659.9	771.8	862.8	907.2	932.5	948.3
C30H16									
1. benzo(e)naphtho(1,2,3,4-ghi)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
2. tetrabenzo(de,hi,mn,qr)tetracene	371.0	373.2	607.4	758.7	886.9	990.7	1041.2	1069.8	1087.7
3. benzo(ghi)naphtho(1,2-e)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
4. benzo(lm)naphtho(1,8-ab)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
5. terrylene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
6. tribenzo(fg,ij,rst)pentaphene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
7. benzo(ghi)naphtho(2,1-e)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
8. phenanthro(1,2,3,4-ghi)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4

Table 10. Standard heat capacity at constant pressure for polycyclic aromatic hydrocarbons in J/K mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
9. benzo(a)peropyrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
10. benzo(ghi)naphtho(1,2-b)perylene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
11. benzo(ghi)naphtho(2,1-a)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
12. tribenzo(a,e,ghi)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
13. dibenzo(e,h)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
14. tribenzo(b,e,ghi)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
15. benzo(ghi)naphtho(2,1-b)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
16. benzo(pqr)naphtho(2,1,8-def)picene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
17. benzo(rst)naphtho(2,1,8-fgh)pentaphene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
18. tribenzo(de,ij,rst)pentaphene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
19. benzo(a)naphtho(2,1,8-cde)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
20. benzo(qr)naphtho(2,1,8,7-fghi)pentacene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
21. benzo(pq)naphtho(8,1,2-cde)picene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
22. benzo(qr)naphtho(2,1,8,7-defg)pentacene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
23. naphtho(8,1,2-fgh)zethrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
24. dibenzo(a,e)arthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
25. benzo(ij)naphtho(2,1,8,7-defg)pentaphene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
26. benzo(de)naphtho(2,1,8,7-ijkl)pentaphene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
28. benzo(a)naphtho(2,1,8-lmn)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
29. naphtho(2,1-e)anthanthrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
30. benzo(a)naphtho(8,1,2-klm)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
31. naphtho(1,2-e)anthanthrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
32. anthra(9,1,2-bcd)perylene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
33. benzo(g,hi)naphtho(8,1,2-cde)picene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
34. phenanthro(3,4,5,6-fghij)pentaphene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
35. tribenzo(a,ghi,k)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
36. benzo(a)naphtho(1,2,3,4-ghi)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
37. tribenzo(a,ghi,k)perylene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
38. naphtho(2,3-e)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
39. benzo(st)naphtho(2,1,8,7-defg)pentacene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
40. anthra(1,2,3,4-ghi)perylene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
43. naphtho(1,2-a)anthanthrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
44. dibenzo(a,n)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
45. naphtho(2,1-a)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
46. pyranthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
48. naphtho(1,2-b)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
49. dibenzo(b,r)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
50. benzo(uv)naphtho(2,1,8,7-defg)pentacene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
51. benzo(de)naphtho(2,1,8,7-qrst)pentacene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
52. benzo(de)naphtho(2,1,8,7-opqr)pentacene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
57. dibenzo(a,k)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
58. dibenzo(b,k)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
59. dibenzo(b,e)anthanthrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
60. naphtho(2,3-a)anthanthrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
61. benzo(uv)naphtho(2,1,8-defg)pentaphene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
62. naphtho(2,1-b)anthanthrene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
63. dinaphtho(8,1,2-cde:2′,1′,8′-hij)naphthacene	375.4	377.5	608.7	759.7	888.3	992.6	1043.5	1072.4	1090.4
67. naphtho(2,3-b)anthanthrene	379.8	381.8	609.9	760.8	889.6	994.4	1045.7	1074.9	1093.2
Coronene series									
C24H12									
1. coronene	290.55	292.36	480.03	598.81	698.69	778.76	817.38	839.09	852.47
C28H14									

Table 10. Standard heat capacity at constant pressure for polycyclic aromatic hydrocarbons in J/K mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
1. dibenzo(hi,qr)anthanthrene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
2. benzo(a)coronene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
3. phenanthro(1,10,9,8-opqra)perylene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
4. naphtho(8,1,2-efg)anthanthrene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
5. dibenzo(cd,hi)anthanthrene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
6. dibenzo(cd,fg)anthanthrene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
7. naphtho(2,1,8-hij)anthanthrene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
9. dibenzo(cd,lm)anthanthrene	343.4	345.4	561.3	699.6	816.5	910.4	955.9	981.5	997.3
C32H16									
1. tribenzo(e,hi,qr)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
2. tribenzo(b,hi,qr)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
3. dibenzo(a,j)coronene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
4. dibenzo(a,g)coronene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
5. dibenzo(a,d)coronene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
6. naphtho(1,2-a)coronene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
7. naphtho(8,1,2-abc)peropyrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
8. tribenzo(b,fg,qr)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
9. tribenzo(a,cd,fg)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
10. tribenzo(a,cd,hi)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
11. benzo(a)naphtho(8,1,2-efg)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
12. benzo(ghi)terrylene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
13. benzo(qr)naphtho(3,2,1-hi)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
14. dibenzo(bc,mn)peropyrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
16. dinaphtho(1,8-ab:8′,1′,2′,3′-fghi)perylene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
17. naphtho(1,2,3,4-ijk)peropyrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
18. dibenzo(ghi,lm)naphtho(1,8-ab)perylene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
19. naphtho(2,1,8-bcd)peropyrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
20. benzo(a)naphtho(2,1,8-cde)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
21. dibenzo(bc,qr)peropyrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
22. tribenzo(e,hi,cp)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
23. tribenzo(b,fg,cp)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
24. benzo(fg)naphtho(1,8-ab)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
26. tribenzo(b,hi,cp)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
27. benzo(b)naphtho(8,1,2-nop)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
28. benzo(hi)naphtho(1,2,3-qr)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
29. naphtho(2,3-a)coronene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
30. benzo(cd)naphtho(1,2,3-hi)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
31. benzo(cd)naphtho(3,2,1-hi)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
32. benzo(cd)naphtho(3,2,1-fg)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
33. tribenzo(a,hi,cp)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
34. tribenzo(cd,fg,k)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
35. tribenzo(cd,hi,k)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
36. benzo(a)naphtho(2,1,8-lmn)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
37. tribenzo(cd,fg,j)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
38. benzo(a)naphtho(8,1,2-nop)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
39. benzo(e)naphtho(2,1,8-hij)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
40. benzo(a)naphtho(2,1,8-hij)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
42. benzo(b)naphtho(2,1,8-lmn)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
43. benzo(lm)naphtho(1,8-ab)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
47. benzo(a)naphtho(8,1,2-klm)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
49. tribenzo(a,fg,cp)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
50. benzo(n)naphtho(8,1,2-bcd)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
51. benzo(b)naphtho(2,1,8-hij)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1
52. benzo(b)naphtho(8,1,2-efg)anthanthrene	391.8	394.1	641.3	799.4	932.9	1040.2	1092.1	1121.3	1139.4
55. benzo(b)naphtho(8,1,2-klm)anthanthrene	396.2	398.5	642.5	800.5	934.3	1042.1	1094.4	1123.9	1142.1

Table 11. Standard entropy for polycyclic aromatic hydrocarbons in J/K mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10									
pyrene	402.2	403.5	539.6	666.4	829.3	1041.6	1204.9	1336.7	1446.3
C20H12									
1. perylene	456.8	458.4	628.3	785.9	987.9	1251.0	1453.1	1616.3	1752.7
2. benzo(e)pyrere	462.5	464.1	634.1	791.7	993.7	1256.7	1458.9	1622.0	1758.4
3. benzo(a)pyrere	468.3	469.9	639.9	797.4	999.4	1262.5	1464.7	1627.8	1764.2
C24H14									
1. dibenzo(fg,op)naphthacene	511.4	513.3	717.1	905.4	1146.5	1460.3	1701.4	1895.9	2058.5
2. naphtho(8,1,2-ghi)chrysene	551.4	553.3	755.9	943.8	1184.5	1497.7	1738.1	1932.1	2094.2
3. benzo(pqr)picene	522.9	524.8	728.6	916.9	1158.0	1471.8	1712.9	1907.4	2070.0
4. dibenzo(a,e)pyrene	522.9	524.8	728.6	916.9	1158.0	1471.8	1712.9	1907.4	2070.0
5. benzo(b)perylene	522.9	524.8	728.6	916.9	1158.0	1471.8	1712.9	1907.4	2070.0
6. zethrene	517.1	519.1	722.8	911.1	1152.2	1466.1	1707.1	1901.7	2064.2
7. benzo(a)perylene	551.4	553.3	755.9	943.8	1184.5	1497.7	1738.1	1932.1	2094.2
8. dibenzo(b,def)chrysene	517.1	519.1	722.8	911.1	1152.2	1466.1	1707.1	1901.7	2064.2
9. dibenzo(def,p)chrysene	551.4	553.3	755.9	943.8	1184.5	1497.7	1738.1	1932.1	2094.2
10. dibenzo(de,cr)naphthacene	517.1	519.1	722.8	911.1	1152.2	1466.1	1707.1	1901.7	2064.2
11. dibenzo(c,mno)chrysene	551.4	553.3	755.9	943.8	1184.5	1497.7	1738.1	1932.1	2094.2
12. benzo(rst)pentaphene	517.1	519.1	722.8	911.1	1152.2	1466.1	1707.1	1901.7	2064.2
14. naphtho(2,1,8-qra)naphthacene	522.9	524.8	728.6	916.9	1158.0	1471.8	1712.9	1907.4	2070.0
C28H16									
1. tribenzo(f,ij,no)tetraphene	628.7	630.9	866.1	1084.4	1363.8	1727.1	2005.9	2230.6	2418.5
2. tribenzo(a,fg,op)tetracene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
4. naphtho(2,1,8-def)picene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
5. dibenzo(a,pqr)picene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
6. benzo(a)naphtho(8,1,2-fgh)tetracene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
7. naphtho(1,2,3,4-bqr)picene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
8. naphtho(1,2-b)perylene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
9. naphtho(2,1-a)perylene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
10. dibenzo(j,pcr)picene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
11. benzo(fg)naphtho(3,2,1-op)tetracene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
12. tribenzo(f,m,pqr)tetraphene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
13. dibenzo(f,pcr)picene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
14. tribenzo(a,hi,mn)tetracene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
15. naphtho(1,2-e)perylene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
16. dibenzo(a,e)perylene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
17. dibenzo(fg,cr)pentacene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
18. naphtho(8,1,2-cde)picene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
19. benzo(c)naphtho(8,1,2-ghi)tetraphene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
20. benzo(a)zethrene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
21. dibenzo(de,kl)pentaphene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
23. dibenzo(a,n)perylene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
25. dibenzo(de,ij)pentaphene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
26. benzo(f)zethrene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
27. dibenzo(a,j)perylene	628.7	630.9	866.1	1084.4	1363.8	1727.1	2005.9	2230.6	2418.5
28. dibenzo(h,rst)pentaphene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
29. dibenzo(b,tuv)picene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8

Table 11. Standard entropy for polycyclic aromatic hydrocarbons in J/K mol continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
30. dibenzo(b,j)perylene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
31. dibenzo(fg,ij)pentaphene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
32. phrenthro(1,2,3,4-pqr)tetracene	634.5	636.7	871.9	1090.1	1369.5	1732.8	2011.6	2236.4	2424.2
33. benzo(c)naphtho(1,2,3,4-pqr)tetracene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
34. dibenzo(b,c)perylene	600.2	602.5	838.8	1057.5	1337.3	1701.2	1980.6	2206.0	2394.3
37. naphtho(2,1,8-fgh)pentacene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
38. dibenzo(fg,st)pentaphene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
39. benzo(de)naphtho(1,2,3-qr)tetracene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
40. dibenzo(de,uv)pentaphene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
43. benzo(c)naphthol(8,1,2-mno)tetraphene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
44. naphtho(8,1,2-cde)pentaphene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
45. tribenzo(c,m,pqr)tetraphene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
46. naphtho(8,1,2-opq)pentacene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
47. dibenzo(o,rst)pentaphene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
49. naphtho(1,2,3,4-rst)pentaphene	628.7	630.9	866.1	1084.4	1363.8	1727.1	2005.9	2230.6	2418.5
50. dibenzo(c,rst)pentaphene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
52. benzo(a)naphtho(2,1,8-hij)tetracene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
53. benzo(a)naphtho(8,1,2-cde)tetracene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
54. dibenzo(de,st)pentacene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
55. dibenzo(de,qr)pentacene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
56. heptazethrene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
59. naphtho(2,3-a)perylene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
60. dibenzo(a,f)perylene	628.7	630.9	866.1	1084.4	1363.8	1727.1	2005.9	2230.6	2418.5
61. benzo(vwx)hexaphene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
62. anthra 2,1,9-qra)tetracene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
63. phenanthro(9,10,1-hif)tetracene	606.0	608.2	844.6	1063.2	1343.1	1707.0	1986.4	2211.7	2400.0
64. dibenzo(de,uv)pentacene	571.7	574.0	811.6	1030.6	1310.8	1675.4	1955.4	2181.3	2370.1
65. benzo(a)naphtho(8,1,2-lmn)tetracene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
68. naphtho(2,1,8-jkl)pentacene	577.5	579.8	817.3	1036.3	1316.6	1681.2	1961.2	2187.0	2375.8
Naphthopyrene series									
C22H12									
1. benzo(ghi)perylene	477.75	479.45	662.23	832.05	1049.18	1331.04	1547.07	1721.11	1866.44
3. dibenzo(def,mno)chrysene	477.75	479.45	662.23	832.05	1049.18	1331.04	1547.07	1721.11	1866.44
C26H14									
1. dibenzo(e,ghi)perylene	538.1	540.1	756.7	957.3	1213.5	1546.1	1801.1	2006.5	2178.0
2. naphtho(1,2,3,4-ghi)perylene	532.3	534.4	751.0	951.5	1207.8	1540.4	1795.3	2000.7	2172.2
3. dibenzo(cd,lm)perylene	526.6	528.6	745.2	945.7	1202.0	1534.6	1789.6	1995.0	2166.5
4. dibenzo(b,ghi)perylene	538.1	540.1	756.7	957.3	1213.5	1546.1	1801.1	2006.5	2178.0
5. naphtho(8,1,2-bcd)perylene	538.1	540.1	756.7	957.3	1213.5	1546.1	1801.1	2006.5	2178.0
6. benzo(e)anthanthrene	538.1	540.1	756.7	957.3	1213.5	1546.1	1801.1	2006.5	2178.0
7. dibenzo(a,ghi)perylene	566.6	568.6	784.0	984.2	1240.0	1572.0	1826.3	2031.2	2202.2
8. benzo(a)anthanthrene	538.1	540.1	756.7	957.3	1213.5	1546.1	1801.1	2006.5	2178.0
10. benzo(b)anthanthrene	538.1	540.1	756.7	957.3	1213.5	1546.1	1801.1	2006.5	2178.0
C30H16									
1. benzo(e)naphtho(1,2,3,4-ghi)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
2. tetrabenzo(de,hi,mn,qr)tetracene	638.2	640.5	888.5	1119.0	1413.5	1795.6	2088.3	2324.0	2520.7
3. benzo(ghi)naphtho(1,2-e)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
4. benzo(lm)naphtho(1,8-ab)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
5. terrylene	581.2	583.5	834.0	1065.2	1360.6	1744.0	2037.8	2274.6	2472.3
6. tribenzo(fg,ij,rst)pentaphene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
7. benzo(ghi)naphtho(2,1-e)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
8. phenanthro(1,2,3,4-ghi)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0

Table 11. Standard entropy for polycyclic aromatic hydrocarbons in J/K mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
9. benzo(a)peropyrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
10. benzo(ghi)naphtho(1,2-b)perylene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
11. benzo(ghi)naphtho(2,1-a)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
12. tribenzo(a,e,ghi)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
13. dibenzo(e,h)anthanthrene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
14. tribenzo(b,e,ghi)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
15. benzo(ghi)naphtho(2,1-b)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
16. benzo(pqr)naphtho(2,1,8-def)picene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
17. benzo(rst)naphtho(2,1,8-fgh)pentaphene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
18. tribenzo(de,ij,rst)pentaphene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
19. benzo(a)naphtho(2,1,8-cde)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
20. benzo(qr)naphtho(2,1,8,7-fghi)pentacene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
21. benzo(pq)naphtho(8,1,2-cde)picene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
22. benzo(qr)naphtho(2,1,8,7-defg)pentacene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
23. naphtho(8,1,2-fgh)zethrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
24. dibenzo(a,e)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
25. benzo(ij)naphtho(2,1,8,7-defg)pentaphene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
26. benzo(de)naphtho(2,1,8,7-ijkl)pentaphene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
28. benzo(a)naphtho(2,1,8-lmn)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
29. naphtho(2,1-e)anthanthrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
30. benzo(a)naphtho(8,1,2-klm)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
31. naphtho(1,2-e)anthanthrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
32. anthra(9,1,2-bcd)perylene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
33. benzo(g,hi)naphtho(8,1,2-cde)picene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
34. phenanthro(3,4,5,6-fghij)pentaphene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
35. tribenzo(a,ghi,k)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
36. benzo(a)naphtho(1,2,3,4-ghi)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
37. tribenzo(a,ghi,k)perylene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
38. naphtho(2,3-e)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
39. benzo(st)naphtho(2,1,8,7-defg)pentacene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
40. anthra(1,2,3,4-ghi)perylene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
43. naphtho(1,2-a)anthanthrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
44. dibenzo(a,n)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
45. naphtho(2,1-a)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
46. pyranthrene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
48. naphtho(1,2-b)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
49. dibenzo(b,r)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
50. benzo(uv)naphtho(2,1,8,7-defg)pentacene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
51. benzo(de)naphtho(2,1,8,7-qrst)pentacene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
52. benzo(de)naphtho(2,1,8,7-opqr)pentacene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
57. dibenzo(a,k)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
58. dibenzo(b,k)anthanthrene	586.9	589.3	839.7	1071.0	1366.3	1749.7	2043.6	2280.3	2478.1
59. dibenzo(b,e)anthanthrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
60. naphtho(2,3-a)anthanthrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
61. benzo(uv)naphtho(2,1,8-defg)pentaphene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
62. naphtho(2,1-b)anthanthrene	621.2	623.5	872.7	1103.6	1398.6	1781.3	2074.6	2310.8	2508.0
63. dinaphtho(8,1,2-cde:2′,1′,8′-hij)naphthacene	615.4	617.8	867.0	1097.9	1392.8	1775.5	2068.8	2305.0	2502.3
67. naphtho(2,3-b)anthanthrene	592.7	595.1	845.5	1076.7	1372.1	1755.5	2049.3	2286.1	2483.8
Coronene series									
C24H12									
1. coronene	487.18	488.99	684.61	866.68	1098.93	1399.57	1629.48	1814.42	1968.67
C28H14									

Table 11. Standard entropy for polycyclic aromatic hydrocarbons in J/K mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
1. dibenzo(hi,qr)anthanthrene	547.5	549.7	779.1	991.9	1263.3	1614.7	1883.5	2099.8	2280.2
2. benzo(a)coronene	547.5	549.7	779.1	991.9	1263.3	1614.7	1883.5	2099.8	2280.2
3. phenanthro(1,10,9,8-opqra)perylene	541.8	543.9	773.3	986.1	1257.5	1608.9	1877.7	2094.0	2274.5
4. naphtho(8,1,2-efg)anthanthrene	553.3	555.4	784.9	997.7	1269.0	1620.4	1889.3	2105.6	2286.0
5. dibenzo(cd,hi)anthanthrene	553.3	555.4	784.9	997.7	1269.0	1620.4	1889.3	2105.6	2286.0
6. dibenzo(cd,fg)anthanthrene	547.5	549.7	779.1	991.9	1263.3	1614.7	1883.5	2099.8	2280.2
7. naphtho(2,1,8-hij)anthanthrene	547.5	549.7	779.1	991.9	1263.3	1614.7	1883.5	2099.8	2280.2
9. dibenzo(cd,lm)anthanthrene	547.5	549.7	779.1	991.9	1263.3	1614.7	1883.5	2099.8	2280.2
C32H16									
1. tribenzo(e,hi,qr)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
2. tribenzo(b,hi,qr)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
3. dibenzo(a,j)coronene	596.4	598.8	862.1	1105.6	1416.1	1818.3	2126.0	2373.7	2580.3
4. dibenzo(a,g)coronene	602.1	604.6	867.9	1111.3	1421.8	1824.0	2131.8	2379.4	2586.1
5. dibenzo(a,d)coronene	630.6	633.1	895.1	1138.2	1448.3	1849.8	2157.0	2404.1	2610.3
6. naphtho(1,2-a)coronene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
7. naphtho(8,1,2-abc)peropyrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
8. tribenzo(b,fg,qr)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
9. tribenzo(a,cd,fg)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
10. tribenzo(a,cd,hi)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
11. benzo(a)naphtho(8,1,2-efg)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
12. benzo(ghi)terrylene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
13. benzo(qr)naphtho(3,2,1-hi)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
14. dibenzo(bc,mn)peropyrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
16. dinaphtho(1,8-ab:8′,1′,2′,3′-fghi)perylene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
17. naphtho(1,2,3,4-ijk)peropyrene	602.1	604.6	867.9	1111.3	1421.8	1824.0	2131.8	2379.4	2586.1
18. dibenzo(ghi,lm)naphtho(1,8-ab)perylene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
19. naphtho(2,1,8-bcd)peropyrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
20. benzo(a)naphtho(2,1,8-cde)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
21. dibenzo(bc,qr)peropyrene	602.1	604.6	867.9	1111.3	1421.8	1824.0	2131.8	2379.4	2586.1
22. tribenzo(e,hi,op)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
23. tribenzo(b,fg,op)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
24. benzo(fg)naphtho(1,8-ab)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
26. tribenzo(b,hi,op)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
27. benzo(b)naphtho(8,1,2-nop)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
28. benzo(hi)naphtho(1,2,3-qr)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
29. naphtho(2,3-a)coronene	602.1	604.6	867.9	1111.3	1421.8	1824.0	2131.8	2379.4	2586.1
30. benzo(cd)naphtho(1,2,3-hi)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
31. benzo(cd)naphtho(3,2,1-hi)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
32. benzo(cd)naphtho(3,2,1-fg)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
33. tribenzo(a,hi,op)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
34. tribenzo(cd,fg,k)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
35. tribenzo(cd,hi,k)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
36. benzo(a)naphtho(2,1,8-lmn)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
37. tribenzo(cd,fg,j)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
38. benzo(a)naphtho(8,1,2-nop)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
39. benzo(e)naphtho(2,1,8-hij)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
40. benzo(a)naphtho(2,1,8-hij)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
42. benzo(b)naphtho(2,1,8-lmn)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
43. benzo(lm)naphtho(1,8-ab)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
47. benzo(a)naphtho(8,1,2-klm)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
49. tribenzo(a,fg,op)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
50. benzo(n)naphtho(8,1,2-bcd)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
51. benzo(b)naphtho(2,1,8-hij)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8
52. benzo(b)naphtho(8,1,2-efg)anthanthrene	636.4	638.8	900.9	1144.0	1454.1	1855.6	2162.7	2409.9	2616.0
55. benzo(b)naphtho(8,1,2-klm)anthanthrene	607.9	610.4	873.6	1117.1	1427.6	1829.8	2137.5	2385.2	2591.8

Table 12. Standard enthalpy of formation for polycyclic aromatic hydrocarbons in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10									
pyrene	230.5	230.4	218.1	211.0	206.7	208.2	212.6	216.1	217.0
C20H12									
1. perylene	279.9	279.7	265.7	257.7	253.2	256.0	262.4	267.6	269.6
2. benzo(e)pyrene	279.9	279.7	265.7	257.7	253.2	256.0	262.4	267.6	269.6
3. benzo(a)pyrene	289.1	288.9	274.9	266.9	262.4	265.3	271.6	276.8	278.8
C24H14									
1. dibenzo(fg,op)naphthacene	329.2	329.1	313.3	304.4	299.7	303.9	312.3	319.2	322.2
2. naphtho(8,1,2-ghi)chrysene	351.2	351.1	334.8	325.7	320.7	324.1	331.4	337.1	338.8
3. benzo(pqr)picene	347.7	347.5	331.7	322.8	318.1	322.3	330.7	337.6	340.6
4. dibenzo(a,e)pyrene	338.5	338.3	322.5	313.6	308.9	313.1	321.5	328.4	331.4
5. benzo(b)perylene	338.5	338.3	322.5	313.6	308.9	313.1	321.5	328.4	331.4
6. zethrene	347.7	347.5	331.7	322.8	318.1	322.3	330.7	337.6	340.6
7. benzo(a)perylene	351.2	351.1	334.8	325.7	320.7	324.1	331.4	337.1	338.8
8. dibenzo(b,def)chrysene	347.7	347.5	331.7	322.8	318.1	322.3	330.7	337.6	340.6
9. dibenzo(def,p)chrysene	351.2	351.1	334.8	325.7	320.7	324.1	331.4	337.1	338.8
10. dibenzo(de,qr)naphthacene	347.7	347.5	331.7	322.8	318.1	322.3	330.7	337.6	340.6
11. dibenzo(c,mno)chrysene	360.5	360.3	344.0	334.9	329.9	333.3	340.6	346.3	348.0
12. benzo(rst)pentaphene	347.7	347.5	331.7	322.8	318.1	322.3	330.7	337.6	340.6
14. naphtho(2,1,3-qra)naphthacene	356.9	356.7	340.9	332.0	327.3	331.6	339.9	346.8	349.8
C28H16									
1. tribenzo(f,ij,no)tetraphene	413.4	413.2	394.7	384.5	379.0	382.9	391.2	397.4	398.8
2. tribenzo(a,fg,op)tetracene	400.6	400.4	382.4	372.4	367.2	372.0	381.3	388.7	391.4
4. naphtho(2,1,8-def)picene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
5. dibenzo(a,pqr)picene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
6. benzo(a)naphtho(8,1,2-fgh)tetracene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
7. naphtho(1,2,3,4-bqr)picene	397.0	396.8	379.3	369.5	364.6	370.2	380.6	389.2	393.2
8. naphtho(1,2-b)perylene	397.0	396.8	379.3	369.5	364.6	370.2	380.6	389.2	393.2
9. naphtho(2,1-a)perylene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
10. dibenzo(j,pqr)picene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
11. benzo(fg)naphtho(3,2,1-op)tetracene	400.6	400.4	382.4	372.4	367.2	372.0	381.3	388.7	391.4
12. tribenzo(f,m,pqr)tetraphene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
13. dibenzo(f,pqr)picene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
14. tribenzo(a,hi,mn)tetracene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
15. naphtho(1,2-e)perylene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
16. dibenzo(a,e)perylene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
17. dibenzo(fg,qr)pentacene	397.0	396.8	379.3	369.5	364.6	370.2	380.6	389.2	393.2
18. naphtho(8,1,2-cde)picene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
19. benzo(c)naphtho(8,1,2-ghi)tetraphene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
20. benzo(a)zethrene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
21. dibenzo(de,kl)pentaphene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
23. dibenzo(a,n)perylene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
25. dibenzo(de,ij)pentaphene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
26. benzo(f)zethrene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
27. dibenzo(a,j)perylene	422.6	422.4	403.9	393.7	388.2	392.1	400.4	406.6	408.0
28. dibenzo(h,rst)pentaphene	397.0	396.8	379.3	369.5	364.6	370.2	380.6	389.2	393.2
29. dibenzo(b,tuv)picene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4

Table 12. Standard enthalpy of formation for polycyclic aromatic hydrocarbons in kJ/mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
30. dibenzo(b,j)perylene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
31. dibenzo(fg,ij)pentaphene	397.0	396.8	379.3	369.5	364.6	370.2	380.6	389.2	393.2
32. phrenthro(1,2,3,4-pqr)tetracene	422.6	422.4	403.9	393.7	388.2	392.1	400.4	406.6	408.0
33. benzo(c)naphtho(1,2,3,4-pqr)tetracene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
34. dibenzo(b,c)perylene	409.8	409.6	391.6	381.6	376.4	381.2	390.5	397.9	400.6
37. naphtho(2,1,8-fgh)pentacene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
38. dibenzo(fg,st)pentaphene	397.0	396.8	379.3	369.5	364.6	370.2	380.6	389.2	393.2
39. benzo(de)naphtho(1,2,3-qr)tetracene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
40. dibenzo(de,uv)pentaphene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
43. benzo(c)naphthol(8,1,2-mno)tetraphene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
44. naphtho(8,1,2-cde)pentaphene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
45. tribenzo(c,m,pqr)tetraphene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
46. naphtho(8,1,2-opq)pentacene	428.2	428.0	410.0	400.0	394.8	399.6	408.9	416.3	419.0
47. dibenzo(o,rst)pentaphene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
49. naphtho(1,2,3,4-rst)pentaphene	422.6	422.4	403.9	393.7	388.2	392.1	400.4	406.6	408.0
50. dibenzo(c,rst)pentaphene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
52. benzo(a)naphtho(2,1,8-hij)tetracene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
53. benzo(a)naphtho(8,1,2-cde)tetracene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
54. dibenzo(de,st)pentacene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
55. dibenzo(de,qr)pentacene	406.2	406.0	388.5	378.7	373.8	379.4	389.8	398.4	402.4
56. heptazethrene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
59. naphtho(2,3-a)perylene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
60. dibenzo(a,f)perylene	422.6	422.4	403.9	393.7	388.2	392.1	400.4	406.6	408.0
61. benzo(vwx)hexaphene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
62. anthra 2,1,9-qra)tetracene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
63. phenanthro(9,10,1-hif)tetracene	419.0	418.8	400.8	390.8	385.6	390.4	399.7	407.1	409.8
64. dibenzo(de,uv)pentacene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
65. benzo(a)naphtho(8,1,2-lmn)tetracene	415.4	415.2	397.7	387.9	383.1	388.6	399.0	407.6	411.7
68. naphtho(2,1,8-jkl)pentacene	424.6	424.4	406.9	397.1	392.3	397.9	408.2	416.8	420.9
Naphthopyrene series									
C22H12									
1. benzo(ghi)perylene	301.29	301.13	287.53	280.17	276.32	279.45	285.42	289.50	289.66
3. dibenzo(def,mno)chrysene	310.50	310.34	296.73	289.38	285.52	288.65	294.62	298.70	298.87
C26H14									
1. dibenzo(e,ghi)perylene	350.7	350.5	335.1	326.9	322.8	327.3	335.3	341.1	342.3
2. naphtho(1,2,3,4-ghi)perylene	350.7	350.5	335.1	326.9	322.8	327.3	335.3	341.1	342.3
3. dibenzo(cd,lm)perylene	359.9	359.7	344.3	336.1	332.0	336.5	344.5	350.3	351.5
4. dibenzo(b,ghi)perylene	359.9	359.7	344.3	336.1	332.0	336.5	344.5	350.3	351.5
5. naphtho(8,1,2-bcd)perylene	359.9	359.7	344.3	336.1	332.0	336.5	344.5	350.3	351.5
6. benzo(e)anthanthrene	359.9	359.7	344.3	336.1	332.0	336.5	344.5	350.3	351.5
7. dibenzo(a,ghi)perylene	372.7	372.5	356.7	348.2	343.8	347.5	354.4	359.0	358.9
8. benzo(a)anthanthrene	369.1	368.9	353.5	345.3	341.2	345.7	353.7	359.5	360.7
10. benzo(b)anthanthrene	369.1	368.9	353.5	345.3	341.2	345.7	353.7	359.5	360.7
C30H16									
1. benzo(e)naphtho(1,2,3,4-ghi)perylene	412.8	412.6	395.1	385.7	381.1	386.2	395.0	401.3	402.3
2. tetrabenzo(de,hi,mn,qr)tetracene	434.8	434.6	416.6	407.0	402.1	406.3	414.2	419.2	418.9
3. benzo(ghi)naphtho(1,2-e)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
4. benzo(lm)naphtho(1,8-ab)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
5. terrylene	409.2	409.0	391.9	382.8	378.5	384.4	394.3	401.8	404.1
6. tribenzo(fg,ij,rst)pentaphene	400.0	399.8	382.7	373.6	369.3	375.2	385.1	392.6	394.9
7. benzo(ghi)naphtho(2,1-e)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
8. phenanthro(1,2,3,4-ghi)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5

Table 12. Standard enthalpy of formation for polycyclic aromatic hydrocarbons in kJ/mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
9. benzo(a)peropyrene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
10. benzo(ghi)naphtho(1,2-b)perylene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
11. benzo(ghi)naphtho(2,1-a)perylene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
12. tribenzo(a,e,ghi)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
13. dibenzo(e,h)anthanthrene	409.2	409.0	391.9	382.8	378.5	384.4	394.3	401.8	404.1
14. tribenzo(b,e,ghi)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
15. benzo(ghi)naphtho(2,1-b)perylene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
16. benzo(pqr)naphtho(2,1,8-def)picene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
17. benzo(rst)naphtho(2,1,8-fgh)pentaphene	409.2	409.0	391.9	382.8	378.5	384.4	394.3	401.8	404.1
18. tribenzo(de,ij,rst)pentaphene	409.2	409.0	391.9	382.8	378.5	384.4	394.3	401.8	404.1
19. benzo(a)naphtho(2,1,8-cde)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
20. benzo(qr)naphtho(2,1,8,7-fghi)pentacene	409.2	409.0	391.9	382.8	378.5	384.4	394.3	401.8	404.1
21. benzo(pq)naphtho(8,1,2-cde)picene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
22. benzo(qr)naphtho(2,1,8,7-defg)pentacene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
23. naphtho(8,1,2-fgh)zethrene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
24. dibenzo(a,e)anthanthrene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
25. benzo(ij)naphtho(2,1,8,7-defg)pentaphene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
26. benzo(de)naphtho(2,1,8,7-ijkl)pentaphene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
28. benzo(a)naphtho(2,1,8-lmn)perylene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
29. naphtho(2,1-e)anthanthrene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
30. benzo(a)naphtho(8,1,2-klm)perylene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
31. naphtho(1,2-e)anthanthrene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
32. anthra(9,1,2-bcd)perylene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
33. benzo(g,hi)naphtho(8,1,2-cde)picene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
34. phenanthro(3,4,5,6-fghij)pentaphene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
35. tribenzo(a,ghi,k)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
36. benzo(a)naphtho(1,2,3,4-ghi)perylene	422.0	421.8	404.3	394.9	390.3	395.4	404.3	410.5	411.5
37. tribenzo(a,ghi,k)perylene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
38. naphtho(2,3-e)anthanthrene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
39. benzo(st)naphtho(2,1,8,7-defg)pentacene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
40. anthra(1,2,3,4-ghi)perylene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
43. naphtho(1,2-a)anthanthrene	440.4	440.2	422.7	413.3	408.7	413.8	422.7	428.9	429.9
44. dibenzo(a,n)anthanthrene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
45. naphtho(2,1-a)anthanthrene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
46. pyranthrene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
48. naphtho(1,2-b)anthanthrene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
49. dibenzo(b,r)anthanthrene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
50. benzo(uv)naphtho(2,1,8,7-defg)pentacene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
51. benzo(de)naphtho(2,1,8,7-qrst)pentacene	418.4	418.2	401.1	392.0	387.7	393.6	403.6	411.0	413.3
52. benzo(de)naphtho(2,1,8,7-opqr)pentacene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
57. dibenzo(a,k)anthanthrene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
58. dibenzo(b,k)anthanthrene	427.6	427.4	410.3	401.2	396.9	402.8	412.8	420.2	422.5
59. dibenzo(b,e)anthanthrene	431.2	431.0	413.5	404.1	399.5	404.6	413.5	419.7	420.7
60. naphtho(2,3-a)anthanthrene	422.8	422.6	405.1	395.7	391.1	396.2	405.1	411.4	412.3
61. benzo(uv)naphtho(2,1,8-defg)pentaphene	422.8	422.6	405.1	395.7	391.1	396.2	405.1	411.4	412.3
62. naphtho(2,1-b)anthanthrene	422.8	422.6	405.1	395.7	391.1	396.2	405.1	411.4	412.3
63. dinaphtho(8,1,2-cde:2′,1′,8′-hij)naphthacene	440.4	440.2	422.7	413.3	408.7	413.8	422.7	428.9	429.9
67. naphtho(2,3-b)anthanthrene	436.8	436.6	419.5	410.4	406.1	412.0	422.0	429.4	431.7
Coronene series									
C24H12									
1. coronene	322.70	322.54	309.40	302.66	299.41	302.84	308.40	311.37	309.74
C28H14									

Table 12. Standard enthalpy of formation for polycyclic aromatic hydrocarbons in kJ/mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
1. diberzo(hi,qr)anthanthrene	372.1	371.9	357.0	349.3	345.9	350.7	358.3	362.9	362.4
2. benzc(a)coronene	372.1	371.9	357.0	349.3	345.9	350.7	358.3	362.9	362.4
3. phenanthro(1,10,9,8-opqra)perylene	372.1	371.9	357.0	349.3	345.9	350.7	358.3	362.9	362.4
4. naphtho(8,1,2-efg)anthanthrene	372.1	371.9	357.0	349.3	345.9	350.7	358.3	362.9	362.4
5. diberzo(cd,hi)anthanthrene	381.3	381.1	366.2	358.6	355.1	359.9	367.5	372.1	371.6
6. diberzo(cd,fg)anthanthrene	372.1	371.9	357.0	349.3	345.9	350.7	358.3	362.9	362.4
7. naphtho(2,1,8-hij)anthanthrene	381.3	381.1	366.2	358.6	355.1	359.9	367.5	372.1	371.6
9. diberzo(cd,lm)anthanthrene	390.5	390.3	375.4	367.8	364.3	369.1	376.7	381.3	380.8
C32H16									
1. tribenzo(e,hi,qr)anthanthrene	434.2	434.0	416.9	408.2	404.2	409.6	418.0	423.2	422.4
2. tribenzo(b,hi,qr)anthanthrene	421.4	421.2	404.6	396.0	392.4	398.6	408.1	414.5	415.0
3. diberzo(a,j)coronene	421.4	421.2	404.6	396.0	392.4	398.6	408.1	414.5	415.0
4. diberzo(a,g)coronene	421.4	421.2	404.6	396.0	392.4	398.6	408.1	414.5	415.0
5. diberzo(a,d)coronene	416.6	416.4	399.4	390.6	386.6	392.0	400.5	405.6	404.8
6. naphtho(1,2-a)coronene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
7. naphtho(8,1,2-abc)peropyrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
8. tribenzo(b,fg,qr)anthanthrene	421.4	421.2	404.6	396.0	392.4	398.6	408.1	414.5	415.0
9. tribenzo(a,cd,fg)anthanthrene	421.4	421.2	404.6	396.0	392.4	398.6	408.1	414.5	415.0
10. tribenzo(a,cd,hi)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
11. benzo(a)naphtho(8,1,2-efg)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
12. benzo(ghi)terrylene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
13. benzo(qr)naphtho(3,2,1-hi)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
14. dibenzo(bc,mn)peropyrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
16. dinaphtho(1,8-ab:8′,1′,2′,3′-fghi)perylene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
17. naphtho(1,2,3,4-ijk)peropyrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
18. dibenzo(ghi,lm)naphtho[1,8-ab)perylene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
19. naphtho(2,1,8-bcd)peropyrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
20. benzo(a)naphtho(2,1,8-cde)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
21. dibenzo(bc,qr)peropyrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
22. tribenzo(e,hi,op)anthanthrene	434.2	434.0	416.9	408.2	404.2	409.6	418.0	423.2	422.4
23. tribenzo(b,fg,op)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
24. benzo(fg)naphtho(1,8-ab)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
26. tribenzo(b,hi,op)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
27. benzo(b)naphtho(8,1,2-nop)anthanthrene	430.6	430.4	413.8	405.2	401.6	407.8	417.3	423.7	424.2
28. benzo(hi)naphtho(1,2,3-qr)anthanthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
29. naphtho(2,3-a)coronene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
30. benzo(cd)naphtho(1,2,3-hi)anthanthrene	452.6	452.4	435.3	426.6	422.6	428.0	436.4	441.6	440.8
31. benzo(cd)naphtho(3,2,1-hi)anthanthrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
32. benzo(cd)naphtho(3,2,1-fg)anthanthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
33. tribenzo(a,hi,op)anthanthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
34. tribenzo(cd,fg,k)anthanthrene	434.2	434.0	416.9	408.2	404.2	409.6	418.0	423.2	422.4
35. tribenzo(cd,hi,k)anthanthrene	434.2	434.0	416.9	408.2	404.2	409.6	418.0	423.2	422.4
36. benzo(a)naphtho(2,1,8-lmn)antharthrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
37. tribenzo(cd,fg,j)anthanthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
38. benzo(a)naphtho(8,1,2-nop)antharthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
39. benzo(e)naphtho(2,1,8-hij)antharthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
40. benzo(a)naphtho(2,1,8-hij)antharthrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
42. benzo(b)naphtho(2,1,8-lmn)antharthrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
43. benzo(lm)naphtho(1,8-ab)anthantrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
47. benzo(a)naphtho(8,1,2-klm)antharthrene	449.0	448.8	432.2	423.7	420.0	426.2	435.7	442.1	442.6
49. tribenzo(a,fg,op)anthanthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
50. benzo(n)naphtho(8,1,2-bcd)antharthrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
51. benzo(b)naphtho(2,1,8-hij)antharthrene	439.8	439.6	423.0	414.4	410.8	417.0	426.5	432.9	433.4
52. benzo(b)naphtho(8,1,2-efg)antharthrene	443.4	443.2	426.1	417.4	413.4	418.8	427.2	432.4	431.6
55. benzo(b)naphtho(8,1,2-klm)antharthrene	449.0	448.8	432.2	423.7	420.0	426.2	435.7	442.1	442.6

Table 13. Standard Gibbs energy for polycyclic aromatic hydrocarbons in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Pyrene series									
C16H10									
pyrene	332.8	333.4	405.9	482.5	599.8	796.3	991.7	1187.3	1379.9
C20H12									
1. perylene	411.7	412.5	505.3	602.8	751.8	1000.7	1248.0	1495.3	1738.8
2. benzo(e)pyrene	410.0	410.8	502.4	598.8	746.0	992.1	1236.5	1480.9	1721.5
3. benzo(a)pyrene	417.5	418.3	508.3	603.9	749.4	992.7	1234.2	1475.7	1713.4
C24H14									
1. dibenzo(fg,op)naphthacene	490.6	491.6	604.7	723.1	903.7	1205.2	1504.4	1803.3	2097.7
2. naphtho(8,1,2-ghi)chrysene	500.7	501.6	606.9	717.5	886.7	1169.3	1450.0	1730.7	2007.1
3. benzo(pqr)picene	505.6	506.5	617.4	733.5	910.6	1206.3	1499.7	1792.9	2081.5
4. dibenzo(a,e)pyrene	496.4	497.3	608.2	724.3	901.4	1197.1	1490.5	1783.7	2072.3
5. benzo(b)perylene	496.4	497.3	608.2	724.3	901.4	1197.1	1490.5	1783.7	2072.3
6. zethrene	507.3	508.3	620.3	737.5	916.4	1215.0	1511.3	1807.3	2098.8
7. benzo(a)perylene	500.7	501.6	606.9	717.5	886.7	1169.3	1450.0	1730.7	2007.1
8. dibenzo(b,def)chrysene	507.3	508.3	620.3	737.5	916.4	1215.0	1511.3	1807.3	2098.8
9. dibenzo(def,p)chrysene	500.7	501.6	606.9	717.5	886.7	1169.3	1450.0	1730.7	2007.1
10. dibenzo(de,qr)naphthacene	507.3	508.3	620.3	737.5	916.4	1215.0	1511.3	1807.3	2098.8
11. dibenzo(c,mno)chrysene	509.9	510.8	616.1	726.8	895.9	1178.5	1459.2	1739.9	2016.3
12. benzo(rst)pentaphene	507.3	508.3	620.3	737.5	916.4	1215.0	1511.3	1807.3	2098.8
14. naphtho(2,1,8-qra)naphthacene	514.8	515.7	626.5	742.7	919.8	1215.5	1509.0	1802.1	2090.7
C28H16									
1. tribenzo(f,ij,no)tetraphene	585.6	586.6	707.9	835.2	1029.7	1354.7	1677.3	2000.1	2318.0
2. tribenzo(a,fg,op)tetracene	579.5	580.6	706.3	837.9	1038.7	1373.8	1706.3	2038.7	2366.0
4. naphtho(2,1,8-def)picene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
5. dibenzo(a,pqr)picene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
6. benzo(a)naphtho(8,1,2-fgh)tetracene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
7. naphtho(1,2,3,4-bqr)picene	584.4	585.6	716.8	853.8	1062.6	1410.8	1756.1	2100.9	2440.4
8. naphtho(1,2-b)perylene	584.4	585.6	716.8	853.8	1062.6	1410.8	1756.1	2100.9	2440.4
9. naphtho(2,1-a)perylene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
10. dibenzo(j,pqr)picene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
11. benzo(fg)naphtho(3,2,1-op)tetracene	579.5	580.6	706.3	837.9	1038.7	1373.8	1706.3	2038.7	2366.0
12. tribenzo(f,m,pqr)tetraphene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
13. dibenzo(f,pqr)picene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
14. tribenzo(a,hi,mn)tetracene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
15. naphtho(1,2-e)perylene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
16. dibenzo(a,e)perylene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
17. dibenzo(fg,qr)pentacene	586.2	587.3	719.7	857.8	1068.3	1419.4	1767.6	2115.3	2457.7
18. naphtho(8,1,2-cde)picene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
19. benzo(c)naphtho(8,1,2-ghi)tetraphene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
20. benzo(a)zethrene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
21. dibenzo(de,kl)pentaphene	595.4	596.5	728.9	867.0	1077.5	1428.6	1776.8	2124.5	2466.9
23. dibenzo(a,n)perylene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
25. dibenzo(de,ij)pentaphene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
26. benzo(f)zethrene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
27. dibenzo(a,j)perylene	594.8	595.8	717.1	844.4	1038.9	1363.9	1686.5	2009.3	2327.2
28. dibenzo(h,rst)pentaphene	586.2	587.3	719.7	857.8	1068.3	1419.4	1767.6	2115.3	2457.7
29. dibenzo(b,tuv)picene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6

Table 13. Standard Gibbs energy for polycyclic aromatic hydrocarbons in kJ/mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	3000
30. dibenzo(b,j)perylene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
31. dibenzo(fg,ij)pentaphene	586.2	587.3	719.7	857.8	1068.3	1419.4	1767.6	2115.3	2457.7
32. phrenthro(1,2,3,4-pqr)tetracene	593.0	594.1	714.2	840.4	1033.2	1355.2	1675.0	1994.9	2309.9
33. benzo(c)naphtho(1,2,3,4-pqr)tetracene	588.7	589.9	715.5	847.1	1047.9	1383.0	1715.6	2047.9	2375.2
34. dibenzo(b,c)perylene	590.5	591.6	718.4	851.1	1053.6	1391.6	1727.1	2062.3	2392.5
37. naphtho(2,1,8-fgh)pentacene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
38. dibenzo(fg,st)pentaphene	586.2	587.3	719.7	857.8	1068.3	1419.4	1767.6	2115.3	2457.7
39. benzo(de)naphtho(1,2,3-qr)tetracene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
40. dibenzo(de,uv)pentaphene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
43. benzo(c)naphtho(8,1,2-mno)tetraphene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
44. naphtho(8,1,2-cde)pentaphene	602.9	604.0	735.2	872.2	1081.0	1429.2	1774.5	2119.3	2458.8
45. tribenzo(c,m,pqr)tetraphene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
46. naphtho(8,1,2-cpq)pentacene	607.2	608.3	733.9	865.5	1066.3	1401.4	1734.0	2066.3	2393.6
47. dibenzo(o,rst)pentaphene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
49. naphtho(1,2,3,4-rst)pentaphene	594.8	595.8	717.1	844.4	1038.9	1363.9	1686.5	2009.3	2327.2
50. dibenzo(c,rst)pentaphene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
52. benzo(a)naphtho(2,1,8-hij)tetracene	602.9	604.0	735.2	872.2	1081.0	1429.2	1774.5	2119.3	2458.8
53. benzo(a)naphtho(8,1,2-cde)tetracene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
54. dibenzo(de,st)pentacene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
55. dibenzo(de,qr)pentacene	593.6	594.8	726.0	863.0	1071.8	1420.0	1765.3	2110.1	2449.6
56. heptazethrene	604.6	605.7	738.1	876.2	1086.8	1437.8	1786.0	2133.7	2476.1
59. naphtho(2,3-a)perylene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
60. dibenzo(a,f)perylene	594.8	595.8	717.1	844.4	1038.9	1363.9	1686.5	2009.3	2327.2
61. benzo(vwx)hexaphene	602.9	604.0	735.2	872.2	1081.0	1429.2	1774.5	2119.3	2458.8
62. anthra 2,1,9-qra)tetracene	602.9	604.0	735.2	872.2	1081.0	1429.2	1774.5	2119.3	2458.8
63. phenanthro(9,10,1-hif)tetracene	597.9	599.1	724.7	856.3	1057.1	1392.2	1724.8	2057.1	2384.4
64. dibenzo(de,uv)pentacene	604.6	605.7	738.1	876.2	1086.8	1437.8	1786.0	2133.7	2476.1
65. benzo(a)naphtho(8,1,2-lmn)tetracene	602.9	604.0	735.2	872.2	1081.0	1429.2	1774.5	2119.3	2458.8
68. naphtho(2,1,8-jkl)pentacene	612.1	613.2	744.4	881.4	1090.2	1438.4	1783.7	2128.5	2468.0
Naphthopyrene series									
C22H12									
1. benzo(ghi)perylene	430.28	431.08	521.91	617.13	762.49	1005.20	1246.22	1487.39	1725.09
3. dibenzo(def,mno)chrysene	439.48	440.28	531.11	626.34	771.69	1014.41	1255.43	1496.60	1734.29
C26H14									
1. dibenzo(e,ghi)perylene	507.4	508.4	618.4	733.4	908.7	1201.0	1491.0	1781.0	2066.7
2. naphtho(1,2,3,4-ghi)perylene	509.2	510.1	621.3	737.5	914.5	1209.7	1502.6	1795.4	2084.0
3. dibenzo(cd,lm)perylene	520.1	521.1	633.4	750.7	929.4	1227.5	1523.3	1819.0	2110.5
4. dibenzo(b,ghi)perylene	516.7	517.6	627.6	742.6	917.9	1210.2	1500.3	1790.2	2075.9
5. naphtho(8,1,2-bcd)perylene	516.7	517.6	627.6	742.6	917.9	1210.2	1500.3	1790.2	2075.9
6. benzo(e)anthanthrene	516.7	517.6	627.6	742.6	917.9	1210.2	1500.3	1790.2	2075.9
7. dibenzo(a,ghi)perylene	520.9	521.9	626.4	735.9	903.2	1182.4	1459.7	1737.2	2010.7
8. benzo(a)anthanthrene	525.9	526.8	636.9	751.8	927.1	1219.4	1509.5	1799.4	2085.1
10. benzo(b)anthanthrene	525.9	526.8	636.9	751.8	927.1	1219.4	1509.5	1799.4	2085.1
C30H16									
1. benzo(e)naphtho(1,2,3,4-ghi)perylene	590.6	591.7	716.6	847.1	1046.0	1377.7	1706.9	2036.0	2360.4
2. tetrabenzo(de,hi,mn,qr)tetracene	607.6	608.6	730.2	857.6	1052.0	1376.4	1698.6	2021.0	2338.9
3. benzo(ghi)naphtho(1,2-e)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	2369.6
4. benzo(lm)naphtho(1,8-ab)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	2369.6
5. terrylene	599.0	600.1	732.8	871.0	1081.4	1432.0	1779.7	2127.0	2469.4
6. tribenzo(fg,ij,rst)pentaphene	588.0	589.2	720.7	857.8	1066.4	1414.1	1758.9	2103.4	2442.9
7. benzo(ghi)naphtho(2,1-e)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	2369.6
8. phenanthro(1,2,3,4-ghi)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	2369.6

Table 13. Standard Gibbs energy for polycyclic aromatic hydrocarbons in kJ/mol -- continued

T/K	298	300	500	700	1000	1500	2000	2500	[illegible]
9. benzo(a)peropyrene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	[illegible]
10. benzo(ghi)naphtho(1,2-b)perylene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
11. benzo(ghi)naphtho(2,1-a)perylene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
12. tribenzo(a,e,ghi)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	[illegible]
13. dibenzo(e,h)anthanthrene	597.3	598.4	729.9	867.0	1075.6	1423.3	1768.1	2112.6	[illegible]
14. tribenzo(b,e,ghi)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	[illegible]
15. benzo(ghi)naphtho(2,1-b)perylene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
16. benzo(pqr)naphtho(2,1,8-def)picene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
17. benzo(rst)naphtho(2,1,8-fgh)pentaphene	595.5	596.7	727.1	863.0	1069.9	1414.7	1756.6	2098.2	[illegible]
18. tribenzo(de,ij,rst)pentaphene	595.5	596.7	727.1	863.0	1069.9	1414.7	1756.6	2098.2	[illegible]
19. benzo(a)naphtho(2,1,8-cde)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	[illegible]
20. benzo(qr)naphtho(2,1,8,7-fghi)pentacene	595.5	596.7	727.1	863.0	1069.9	1414.7	1756.6	2098.2	[illegible]
21. benzo(pq)naphtho(8,1,2-cde)picene	615.7	616.8	748.4	885.4	1094.0	1441.7	1786.5	2131.0	[illegible]
22. benzo(qr)naphtho(2,1,8,7-defg)pentacene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
23. naphtho(8,1,2-fgh)zethrene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
24. dibenzo(a,e)anthanthrene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
25. benzo(ij)naphtho(2,1,8,7-defg)pentaphene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
26. benzo(de)naphtho(2,1,8,7-ijkl)pentaphene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
28. benzo(a)naphtho(2,1,8-lmn)perylene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
29. naphtho(2,1-e)anthanthrene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
30. benzo(a)naphtho(8,1,2-klm)perylene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
31. naphtho(1,2-e)anthanthrene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
32. anthra(9,1,2-bcd)perylene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
33. benzo(g,hi)naphtho(8,1,2-cde)picene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
34. phenanthro(3,4,5,6-fghij)pentaphene	606.5	607.6	739.2	876.2	1084.8	1432.5	1777.3	2121.8	[illegible]
35. tribenzo(a,ghi,k)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	[illegible]
36. benzo(a)naphtho(1,2,3,4-ghi)perylene	599.8	600.9	725.8	856.3	1055.2	1386.9	1716.1	2045.2	[illegible]
37. tribenzo(a,ghi,k)perylene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
38. naphtho(2,3-e)anthanthrene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
39. benzo(st)naphtho(2,1,8,7-defg)pentacene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
40. anthra(1,2,3,4-ghi)perylene	606.5	607.6	739.2	876.2	1084.8	1432.5	1777.3	2121.8	[illegible]
43. naphtho(1,2-a)anthanthrene	618.2	619.3	744.2	874.7	1073.6	1405.3	1734.5	2063.6	[illegible]
44. dibenzo(a,n)anthanthrene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
45. naphtho(2,1-a)anthanthrene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
46. pyranthrene	615.7	616.8	748.4	885.4	1094.0	1441.7	1786.5	2131.0	[illegible]
48. naphtho(1,2-b)anthanthrene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
49. dibenzo(b,r)anthanthrene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
50. benzo(uv)naphtho(2,1,8,7-defg)pentacene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
51. benzo(de)naphtho(2,1,8,7-qrst)pentacene	604.7	605.9	736.3	872.2	1079.1	1423.9	1765.8	2107.4	[illegible]
52. benzo(de)naphtho(2,1,8,7-opqr)pentacene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
57. dibenzo(a,k)anthanthrene	613.9	615.1	745.5	881.4	1088.3	1433.1	1775.0	2116.6	[illegible]
58. dibenzo(b,k)anthanthrene	615.7	616.8	748.4	885.4	1094.0	1441.7	1786.5	2131.0	[illegible]
59. dibenzo(b,e)anthanthrene	609.0	610.1	735.0	865.5	1064.4	1396.1	1725.3	2054.4	[illegible]
60. naphtho(2,3-a)anthanthrene	600.7	601.8	726.6	857.1	1056.0	1387.7	1716.9	2046.0	[illegible]
61. benzo(uv)naphtho(2,1,8-defg)pentaphene	600.7	601.8	726.6	857.1	1056.0	1387.7	1716.9	2046.0	[illegible]
62. naphtho(2,1-b)anthanthrene	600.7	601.8	726.6	857.1	1056.0	1387.7	1716.9	2046.0	[illegible]
63. dinaphtho(8,1,2-cde:2',1',8'-hij)naphthacene	620.0	621.1	747.1	878.7	1079.3	1413.9	1746.0	2078.0	[illegible]
67. naphtho(2,3-b)anthanthrene	623.2	624.3	754.7	890.6	1097.5	1442.3	1784.2	2125.8	[illegible]
Coronene series									
C24H12									
1. coronene	452.29	453.09	544.25	639.55	784.75	1026.94	1267.46	1508.31	1745.97
C28H14									

Table 13. Standard Gibbs energy for polycyclic aromatic hydrocarbons in kJ/mol -- continued

T/K	293	300	500	700	1000	1500	2000	2500	3000
1. dibenzo(hi,qr)arthanthrene	529.5	530.4	640.8	755.8	931.0	1222.8	1512.3	1801.9	2087.6
2. benzo(a)coronene	529.5	530.4	640.8	755.8	931.0	1222.8	1512.3	1801.9	2087.6
3. phenanthro(1,10,9,8-opqra)perylene	531.2	532.2	643.7	759.9	936.7	1231.4	1523.8	1816.3	2104.9
4. naphtho(8,1,2-efg)anthanthrene	527.7	528.7	637.9	751.8	925.2	1214.1	1500.8	1787.5	2070.3
5. dibenzo(cd,hi)arthanthrene	536.9	537.9	647.1	761.0	934.4	1223.3	1510.0	1796.7	2079.5
6. dibenzo(cd,fg)arthanthrene	529.5	530.4	640.8	755.8	931.0	1222.8	1512.3	1801.9	2087.6
7. naphtho(2,1,8-hij)anthanthrene	538.7	539.6	650.0	765.1	940.2	1232.0	1521.5	1811.1	2096.8
9. dibenzo(cd,lm)arthanthrene	547.9	548.8	659.2	774.3	949.4	1241.2	1530.7	1820.3	2106.0
C32H16									
1. tribenzo(e,hi,qr)anthanthrene	610.9	612.0	736.0	865.4	1062.4	1390.8	1716.6	2042.5	2363.9
2. tribenzo(b,hi,qr)anthanthrene	606.6	607.8	737.3	872.1	1077.2	1418.6	1757.1	2095.5	2429.2
3. dibenzo(a,j)corcnene	610.1	611.2	743.1	880.2	1088.7	1435.9	1780.2	2124.3	2463.8
4. dibenzo(a,g)corcnene	608.3	609.5	740.2	876.2	1082.9	1427.2	1768.6	2109.9	2446.5
5. dibenzo(a,d)corcnene	595.1	596.2	721.3	851.9	1050.6	1381.9	1710.5	2039.3	2363.7
6. naphtho(1,2-a)ccronene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
7. naphtho(8,1,2-atc)peropyrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
8. tribenzo(b,fg,qr)anthanthrene	606.6	607.8	737.3	872.1	1077.2	1418.6	1757.1	2095.5	2429.2
9. tribenzo(a,cd,fg)anthanthrene	606.6	607.8	737.3	872.1	1077.2	1418.6	1757.1	2095.5	2429.2
10. tribenzo(a,cd,hi)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
11. benzo(a)naphthc(8,1,2-efg)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
12. benzo(ghi)terrylene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
13. benzo(qr)naphtho(3,2,1-hi)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
14. dibenzo(bc,mn)peropyrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
16. dinaphtho(1,8-ab:8′,1′,2′,3′-fghi)perylene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
17. naphtho(1,2,3,4-ijk)peropyrene	617.5	618.7	749.4	885.4	1092.1	1436.4	1777.8	2119.1	2455.7
18. dibenzo(ghi,lm)naphtho(1,8-ab)perylene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
19. naphtho(2,1,8-tcd)peropyrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
20. benzo(a)naphthc(2,1,8-cde)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
21. dibenzo(bc,qr)peropyrene	626.8	627.9	758.6	894.6	1101.3	1445.6	1787.0	2128.3	2464.9
22. tribenzo(e,hi,cp)anthanthrene	610.9	612.0	736.0	865.4	1062.4	1390.8	1716.6	2042.5	2363.9
23. tribenzo(b,fg,cp)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
24. benzo(fg)naphtho(1,8-ab)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
26. tribenzo(b,hi,cp)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
27. benzo(b)naphthc(8,1,2-nop)anthanthrene	615.8	617.0	746.5	881.4	1086.4	1427.8	1766.3	2104.7	2438.4
28. benzo(hi)naphtho(1,2,3-qr)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
29. naphtho(2,3-a)coronene	626.8	627.9	758.6	894.6	1101.3	1445.6	1787.0	2128.3	2464.9
30. benzo(cd)naphtho(1,2,3-hi)anthanthrene	629.3	630.4	754.4	883.8	1080.9	1409.2	1735.0	2060.9	2382.4
31. benzo(cd)naphtho(3,2,1-hi)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
32. benzo(cd)naphtho(3,2,1-fg)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
33. tribenzo(a,hi,cp)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
34. tribenzo(cd,fg,k)anthanthrene	610.9	612.0	736.0	865.4	1062.4	1390.8	1716.6	2042.5	2363.9
35. tribenzo(cd,hi,k)anthanthrene	610.9	612.0	736.0	865.4	1062.4	1390.8	1716.6	2042.5	2363.9
36. benzo(a)naphthc(2,1,8-lmn)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
37. tribenzo(cd,fg,j)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
38. benzo(a)naphthc(8,1,2-nop)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
39. benzo(e)naphtho(2,1,8-hij)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
40. benzo(a)naphthc(2,1,8-hij)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
42. benzo(b)naphthc(2,1,8-lmn)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
43. benzo(lm)naphtho(1,8-ab)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
47. benzo(a)naphthc(8,1,2-klm)anthanthrene	634.2	635.4	764.9	899.8	1104.8	1446.2	1784.7	2123.1	2456.8
49. tribenzo(a,fg,cp)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
50. benzo(n)naphthc(8,1,2-bcd)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
51. benzo(b)naphthc(2,1,8-hij)anthanthrene	625.0	626.2	755.7	890.6	1095.6	1437.0	1775.5	2113.9	2447.6
52. benzo(b)naphthc(8,1,2-efg)anthanthrene	620.1	621.2	745.2	874.6	1071.6	1400.0	1725.8	2051.7	2373.2
55. benzo(b)naphthc(8,1,2-klm)anthanthrene	634.2	635.4	764.9	899.8	1104.8	1446.2	1784.7	2123.1	2456.8

8. Acknowledgments

The calculations in this paper were made using a terminal connected to the IBM 370/3033N in the MIT Computer Center. Programs were written in APL and tables were printed on a Xerox 8700 Printer in the Computer Center. We are indebted to Professor J. R. Dias for many helpful discussions. This research was supported by a grant from the National Institute of Standards and Technology.

9. Nomenclature

C°_{pi}	= standard heat capacity at constant pressure of isomer i, J K^{-1} mol^{-1}
C°_p(I)	= standard heat capacity at constant pressure of isomer group I, J K^{-1} mol^{-1}
$\Delta_f G^\circ_i$	= standard Gibbs energy of formation of isomer i, kJ mol^{-1}
$\Delta_f G^\circ$(I)	= standard Gibbs energy of formation of isomer group I, kJ mol^{-1}
H°(I,T)–H°(I,298.15 K)	= standard enthalpy for isomer groups relative to isomer groups at 298.15 K kJ mol^{-1}
H°(I,T)–H°(I,298.15 K) + $\Delta_f H^\circ$(I,298.15 K)	= standard enthalpy for isomer groups relative to elements at 298.15 K, kJ mol^{-1}
$\Delta_f H^\circ_i$	= standard enthalpy of formation of isomer i, kJ mol^{-1}
$\Delta_f H^\circ$(I)	= standard enthalpy of formation of isomer group, I, kJ mol^{-1}
n_C	= number of carbon atoms in a molecule
n_H	= number of hydrogen atoms in a molecule
N_I	= number of isomers in an isomer group
r_i	= equilibrium mole fraction of species i in an isomer group
S°_i	= standard entropy of isomer i, J K^{-1} mol^{-1}
S°(I)	= standard entropy of isomer group I, J K^{-1} mol^{-1}
TSN	= total symmetry number
y_i	= mole fraction of isomer i within the isomer group
y_I	= mole fraction of isomer group I in a mixture

10. References

[1]R. A. Alberty and A. K. Reif, J. Phys. Chem. Ref. Data **17**, 241 (1988).
[2]J. R. Dias, Accounts Chem. Res. **18**, 241 (1985).
[3]J. R. Dias, J. Macromol. Sci. Chem. **22** (3), 335 (1985).
[4]J. R. Dias, J. Mol. Struct. (Theochem.) **137**, 9 (1986).
[5]J. R. Dias, J. Mol. Struct. (Theochem.) **149**, 213 (1987).
[6]J. R. Dias, "Part A: Benzenoid Hydrocarbons," in *Handbook of Polycyclic Hydrocarbons*, (Elsevier, Amsterdam, 1987).
[7]J. V. Knop, W. Müller, K. Szmanski, and N. Trinajstić, "Computer Generation of Certain Classes of Molecules"; SKTH/Kemija u industriji, Zagreb, 1985.
[8]R. A. Alberty and C. A. Gehrig, J. Phys. Chem. Ref. Data **13**, 1173 (1984).
[9]R. A. Alberty, J. Phys. Chem. Ref. Data **14**, 177 (1985).
[10]R. A. Alberty and C. A. Gehrig, J. Phys. Chem. Ref. Data **14**, 803 (1985).
[11]R. A. Alberty and T. M. Bloomstein, J. Phys. Chem. Ref. Data **14**, 821 (1985).
[12]R. A. Alberty and Y. S. Ha, J. Phys. Chem. Ref. Data **14**, 1107 (1985).
[13]R. A. Alberty and E. Burmenko, J. Phys. Chem. Ref. Data **15**, 1339 (1986).
[14]R. A. Alberty, E. Burmenko, and M. Chung, J. Phys. Chem. Ref. Data **16**, 193 (1987).
[15]R. A. Alberty, M. B. Chung, and T. M. Flood, J. Phys. Chem. Ref. Data **16**, 391 (1987).
[16]B. D. Smith, AIChE J. **5**, 26 (1959).
[17]W. R. Smith and R. W. Missen, *Chemical Reaction Equilibrium Analysis: Theory and Algorithms* (Wiley–Interscience, New York, 1982).
[18]R. A. Alberty, Ind. Eng. Chem. **22**, 318 (1983).
[19]S. W. Benson, *Thermochemical Kinetics* (Wiley, New York, 1976).
[20]S. E. Stein, D. M. Golden, and S. W. Benson, J. Phys. Chem. **81**, 314 (1977).
[21]S. E. Stein and A. Fahr, J. Phys. Chem. **89**, (1985).
[22]B. Nelander and S. J. Sunner, Chem. Phys. **44**, 2476 (1966).
[23]E. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Chruney, and R. L. Nuttall, The NSB tables of chemical thermodynamic properties, J. Phys. Chem. Ref. Data **11**, Suppl. No. 2 (1982).
[24]M. W. Chase, C. A. Davies, J. R. Downey, D. J. Frurip, R. A. McDonald, and A. N. Syverud, JANAF Thermochemical Tables, 3rd ed., J. Phys. Chem. Ref. Data **14**, Suppl. No. 1 (1985).
[25]E. R. Cohen and B. N. Taylor, The 1986 Adjustment of the Fundamental Physical Constants, CODATA Bulletin, No. 63, 1986.
[26]TRC Thermodynamic Tables, Hydrocarbons, Vols. 7 and 8, Thermodynamics Research Center, The Texas A&M University System, College Station, Texas, 1986.
[27]J. B. Pedley, R. D. Naylor, and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed. (Chapman and Hall, New York, 1986).
[28]N. K. Smith, R. C. Stewart, A. G. Osborn, and D. W. Scott, J. Chem. Thermodyn. **12**, 919 (1980).
[29]W. K. Wong and E. F. Westrum, J. Chem. Thermodyn. **3**, 105 (1971).
[30]I. Mills, *Quantities, Units and Symbols in Physical Chemistry* (Blackwell Scientific, Boston, 1988).
[31]*Nomenclature of Organic Chemistry*, edited by J. Rigaudy and S. P. Klesney (Pergamon, New York, 1979).
[32]E. Clar, *Polycyclic Hydrocarbons* (Academic, New York, 1964).
[33]R. A. Alberty and I. Oppenheim, J. Chem. Phys. **89**, 3689 (1988).

11. Appendix Table A.1 Group Additivity Values of Stein and Fahr for Benzenoid Aromatic Hydrocarbons

Group	ΔH°_{298} kJ mol^{-1}	S°_{298} JK^{-1}mol^{-1}	C_p°/J K^{-1} mol^{-1}										
			300	400	500	600	800	1000	1250	1500	2000	2500	3000
C_B-(H)	13.8	48.2	13.8	18.8	23.1	26.6	31.6	35.1	38.2	40.3	42.8	44.2	45
C_{FR}-(C_{FR})(C_B)2	20.1	-20.9	12.6	15.4	17.5	19.3	22	23.7	25	25.8	26.6	27	27.2
C_{FR}-(C_{FR})2(C_B)	15.5	-20.9	12.6	15.4	17.5	19.3	22	23.7	25	25.8	26.6	27	27.2
C_{FR}-(C_{FR})3	6.1	7.6	8.4	13	16.3	18.5	21.1	22.4	23.2	23.7	24.2	24.5	24.6