

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. III. Naphthocoronene Series, Ovalene Series, and First Members of Some Higher Series

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The tables in our first two papers on polycyclic aromatic hydrocarbons [J. Phys. Chem. Ref. Data 17, 241 (1988) and J. Phys. Chem. Ref. Data (18, 77 (1989)], have been extended by calculating thermodynamic properties for the first two isomer groups in the naphthocoronene series, the first two isomer groups in the ovalene series, and first members of some higher series. Successive isomer groups in each series differ by C_4H_2 . 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 $\Delta_f G^\circ$ for a standard state pressure of 1 bar are given for isomer groups and for individual species. 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; naphthocoronene; ovalene; Benson method; enthalpy of formation; heat capacity; isomer group thermodynamic properties; isomer mole fractions; thermodynamic properties.

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1. Introduction

The preceding two articles in this series^{1,2} presented thermodynamic tables for the isomer groups in the first four series of benzenoid polycyclic aromatic hydrocarbons and the individual species. This paper extends these tables to the next two isomer groups and includes first members of the higher series up to C₉₆H₂₄. Some of the needs for thermodynamic properties of polycyclic aromatic hydrocarbons have been indicated in the preceding articles.

Dias³⁻⁸ 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 H₂. Table 1 gives the molecular formulas, numbers of rings, and numbers of isomers for the naphthocoronene and ovalene series and for first members of some higher series for which calculations are presented in this paper. Although it is known⁹ that there are 37 isomers of C₃₄H₁₆, the structures of 20 are available, and are shown in Table 1. Since three of these are diradicals, we have made calculations on only 17 isomers.

In view of the lack of information on the numbers of isomers in successive isomer groups in series beyond the ovalene series, we have concentrated on first members of higher series. The thermodynamic properties of successive isomer groups in these series may be estimated from the properties of the first members and trends in the increments of the series previously studied.

Table 2 gives the formula, numbers of rings, and numbers of isomers for first members of series up to C₉₆H₂₆, which is 2-circumcoronene. The pattern of this table after pyrene (C₁₆H₁₀) is clear. There are two lines of the same length, a single line, then two lines of the same length. We have this pattern continues all the way to an infinite carbon number. Thermodynamic tables are given for first members for only some of the higher series because of lack of information about structures of isomers. However, the thermodynamic tables are complete for first members along the left-hand edge of Table 2. These species are especially important because they are the ones with the lowest H/C ratio. In the series after the coronene series, the H/C ratios increase as C₄H₂ increments are added. Thus the species along the right-hand edge of Table 2 will tend to predominate within their series at equilibrium under conditions where there is a lack of hydrogen.

The structural formulas of the isomers considered in this paper are given in Fig. 1. To simplify this figure only C-C bonds are shown. Isomers of C₃₄H₁₆, numbered 10, 13, and 16 are diradicals (J. R. Dias, personal communication),

and so they were omitted from the calculations.

The tables presented here are of the same type as those published earlier for alkanenes,¹⁰ alkylbenzenes,¹¹ alkenes,¹² alkylnaphthalenes,¹³ alkylcyclopentanes and cyclohexanes,¹⁴ alkynes,¹⁵ thiols,¹⁶ alkanols,¹⁷ benzene-series polycyclic aromatic hydrocarbons,¹ and polycyclic aromatic hydrocarbons in the pyrene, naphthopyrene, and coronene series.²

2. Standard Thermodynamic Properties of Polycyclic Aromatic Isomer Groups

When isomers are in equilibrium, the standard Gibbs energy of formation $\Delta_f G^\circ(\mathbf{I})$ of the isomer groups is defined by^{18,19}

$$\Delta_f G^\circ(\mathbf{I}) = -RT \ln \sum_{i=1}^{N_i} \exp(-\Delta_f G_i^\circ/RT), \quad (1)$$

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 i in the group. The equilibrium mole fractions r_i of various isomers in a group can be calculated using

$$r_i = \frac{y_i}{y_1} = \exp\{[\Delta_f G^\circ(\mathbf{I}) - \Delta_f G_i^\circ]/RT\}, \quad (2)$$

where y_1 is the sum of the mole fractions of the individual isomers. The corresponding equations for the other standard thermodynamic properties $C_p^\circ(\mathbf{I})$, $S^\circ(\mathbf{I})$, and $\Delta_f H^\circ(\mathbf{I})$ can be derived by differentiating Eq. (1) with respect to temperature.²⁰ 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

TABLE 1. Three series of polycyclic aromatic hydrocarbons.^a

n_c	Naphthocoronene series	Ovalene series	First members of some higher series
30	C ₃₀ H ₁₄ (9,3)		
32		C ₃₂ H ₁₄ (10,1)	
34	C ₃₄ H ₁₆ (10,17)		
36		C ₃₆ H ₁₆ (11,20)	
38	C ₃₈ H ₁₈ (11,)		C ₃₈ H ₁₆ (12,10)
40		C ₄₀ H ₁₈ (12,)	C ₄₀ H ₁₆ (13,3)
42			C ₄₂ H ₁₆ (16,1)
54			C ₅₄ H ₁₈ (19,1)
66			C ₆₆ H ₂₀ (24,1)
80			C ₈₀ H ₂₂ (30,1)
96			C ₉₆ H ₂₄ (37,1)

^a The first number in parenthesis is the number of rings and the second is the number of isomers, excluding diradicals.

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TABLE 2. First members of series of polycyclic aromatic hydrocarbons.^a

n_H						
6	$C_6H_6(1,1)$					
8	$C_{10}H_8(2,1)$					
10	$C_{16}H_{10}(4,1)$					
12	$C_{22}H_{12}(6,2)$	$C_{24}H_{12}(7,1)$				
14	$C_{30}H_{14}(9,3)$	$C_{32}H_{14}(10,1)$				
16	$C_{38}H_{16}(12,10)$	$C_{40}H_{16}(13,3)$	$C_{42}H_{16}(16,1)$			
18	$C_{48}H_{18}(16,22)$	$C_{50}H_{18}(17,7)$	$C_{52}H_{18}(18,2)$	$C_{54}H_{18}(19,1)$		
20	$C_{60}H_{20}(21,28)$	$C_{62}H_{20}(22,12)$	$C_{64}H_{20}(23,3)$	$C_{66}H_{20}(24,1)$		
22	$C_{72}H_{22}(26,_)$	$C_{74}H_{22}(27,20)$	$C_{76}H_{22}(28,10)$	$C_{78}H_{22}(29,3)$	$C_{80}H_{22}(30,1)$	
24	$C_{86}H_{24}(32,_)$	$C_{88}H_{24}(33,_)$	$C_{90}H_{24}(34,22)$	$C_{92}H_{24}(35,7)$	$C_{94}H_{24}(36,2)$	$C_{96}H_{24}(37,1)$

^aThe first number in parenthesis is the number of rings and the second number is the number of isomers. The numbers of isomers of some of the higher isomer groups are from Dias (Ref. 8).

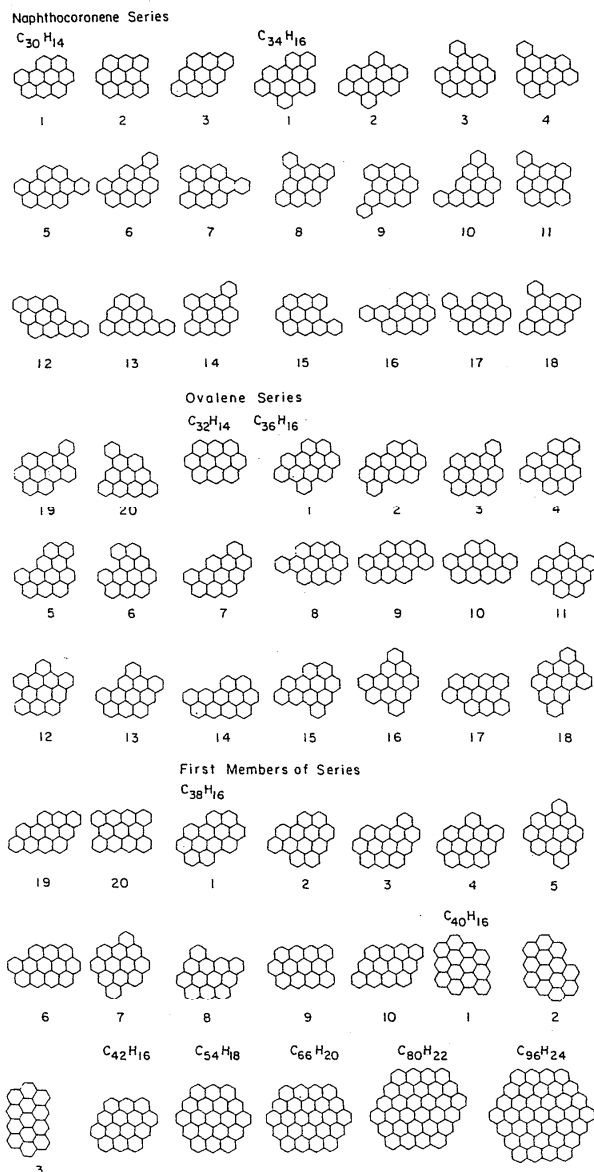


FIG. 1. Structures of isomers in the naphthocoronene series and ovalene series, and first members of some higher series.

thermodynamic properties for an isomer group are interrelated by

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

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 is limited to the smaller molecules. Fortunately enough data were available for Stein, Golden, and Benson^{21,22} to obtain group values for $C_B - (C_{FR} - (C_{FR}))_2$, and $C_{FR} - (C_{FR})_2(C_B)$ groups; group values of $C_{FR} - (C_{FR})_3$ were evaluated from graph. The significance of these symbols is described in Benson's book.²¹ The average difference between predicted and measured $\Delta_f H^\circ(298)$ for eleven polycyclic aromatic hydrocarbons was $< 2 \text{ kcal mol}^{-1}$ and generally was within experimental uncertainties. More recently, Stein and Fahr²³ provided Benson group values with C_p° values up to 300. Although these values are similar to those of Stein, Golden, and Benson,²² 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 $[C_{FR} - (C_{FR})_3]$ group were derived from pyrene frequencies²⁴ 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 already been described.¹ The latest values have been used for various thermodynamic quantities.²⁵⁻²⁷ Comparisons with literature data^{28,29} were given in the preceding two papers. There is a serious shortage of experimental data on polycyclic aromatic hydrocarbons.

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 Naphthocoronene Series, Ovalene Series, and First Members of Some Higher Series

In Tables 3–8 all of the values have been estimated using Benson method. Since the increments from one isomer group to the next are C_4H_2 in each series, the increments in properties are given for each series at each temperature. In the naphthocoronene series and ovalene series, we have been able to make calculations on two isomer groups, which yield the indicated increments in thermodynamic properties per C_4H_2 . For earlier series these increments were found to be a function of temperature only. The increments between first members of series vary because they correspond to C_2 , C_2 , $C_{12}H_2$, $C_{12}H_2$, $C_{14}H_2$, and $C_{16}H_2$, respectively. These increments have a simple interpretation, as given in Sec. 7.

Table 7 gives $H^\circ(I,T) - H^\circ(I,298.15\text{ K})$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H^\circ(I,T) - H^\circ(I,298.15\text{ K}) + \Delta_f H^\circ(I,298.15\text{ K})$, the standard enthalpy for the isomer group relative to the elements at 298.15 K. This quantity is useful for 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 $\Delta_f G^\circ(I)$ and $\Delta_f G^\circ_j$ are about the same, the uncertainty in the difference is nearly independent of the relative values of two parameters, but the absolute uncertainty does increase with temperature.

The substances in the tables are named according to IUPAC, who follows mainly the IUPAC Revised and Collectively Recommended for the Nomenclature of Organic Chemistry, 1978.³¹ The name for $C_{36}H_{16}$ isomer 1 should end with a "rene" at the end, and the name of isomer 15 should end with a "ene" at the end.

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.

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 Benson method for the polycyclic aromatic are given in Tables 10 to 13 in joules for a standard state pressure of 1 bar.

7. Discussion

The circumcoronenes are of special interest because they have the smallest number of hydrogen atoms for a given number of carbon atoms. Thus they are favored at equilibrium at very low hydrogen partial pressures. The molecular formulas for benzene and the circumcoronenes are all represented by $C_{6N}H_{6N}$, where $N = 1$ for benzene, 2 for coronene, 3 for circumcoronene, 4 for 2-circumcoronene, etc. Furthermore, the numbers of Benson groups of various types can also be expressed in terms of N for the circumcoronenes. There are $6N$ $C_B - (H)$ groups, $6(N-1)$ $C_{FR} - (C_{FR})(C_B)_2$ groups, and $6(N-1)^2$ $C_{FR} - (C_{FR})_3$ groups. Thus the standard thermodynamic properties of the circumcoronenes are quadratic functions of N . However, it is perhaps easier to think of them as linear functions of the number of carbon atoms n_C and number of hydrogen atoms n_H . Thus the standard Gibbs energies of formation of these species are represented by

$$\Delta_f G^\circ(I) = a + bn_C + cn_H. \quad (4)$$

Table 14 gives the parameters in this equation determined with $C_{24}H_{12}$, $C_{54}H_{18}$, and $C_{96}H_{24}$. These parameters can be used to calculate standard Gibbs energies of formation of higher circumcoronenes.

There is an error in the values of S° and $\Delta_f G^\circ$ for coronene ($C_{24}H_{12}$) in article II (Ref. 2) because the symmetry number was taken to be 4, rather than 12. The corrected values for the standard entropy of coronene at the temperatures used in this series are 478.0, 479.9, 675.5, 857.5, 1089.8, 1390.4, 1620.3, 1805.3, and 1959.5 $\text{J K}^{-1} \text{mol}^{-1}$. The corrected values for the standard Gibbs energy of formation of coronene are 455.0, 458.8, 548.8, 645.9, 793.9, 1040.6, 1285.7, 1531.1, and 1773.4 kJ mol^{-1} .

Recently Dorofeeva and Gurvich³² have published standard thermodynamic properties of 37 polycyclic aromatic hydrocarbons in the ideal gas phase for 100 and 1500 K. These properties have been calculated statistically mechanically using the rigid rotor, harmonic oscillator approximation and a force-field method to estimate the needed vibrational frequencies. Their values are in general quite close to those calculated in our series of papers using Stein and Fahr²³ parameters in the Benson method.

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 number. It is also convenient to deal with series because the standard thermodynamic properties are very nearly a linear function of the number of C_4H_2 increments added to the first 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.^{33,34} 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 of isomer groups as a single species in an equilibrium calculation.

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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
Naphthocoronene series									
C30H14	360.3	362.5	594.6	740.1	861.6	958.4	1004.8	1030.6	1046.4
C34H16	418.2	420.7	680.9	844.0	980.4	1089.4	1141.8	1171.1	1189.1
Ovalene series									
C32H14	376.2	378.7	626.5	779.1	905.8	1005.8	1053.2	1079.4	1095.2
C36H16	436.4	439.0	711.2	881.9	1024.4	1137.4	1191.2	1221.1	1239.2
Leading members of series									
C38H16	448.0	451.0	744.0	922.8	1070.4	1186.4	1241.1	1271.2	1289.4
C40H16	462.4	465.6	773.7	960.1	1113.3	1233.1	1289.2	1319.8	1338.0
C42H16	478.4	481.8	805.6	999.2	1157.5	1280.5	1337.7	1368.6	1386.9
C54H18	597.0	601.5	1017.4	1259.0	1453.8	1602.9	1670.8	1706.8	1727.5
C66H20	715.5	721.2	1229.1	1518.8	1750.2	1925.3	2004.0	2045.0	2068.2
C80H22	850.6	857.6	1473.5	1818.3	2091.2	2295.3	2385.8	2432.1	2457.7
C96H24	1002.0	1010.6	1750.5	2157.6	2476.8	2713.1	2816.2	2868.2	2896.3

Table 3a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C34-C30	57.9	58.2	86.3	103.9	118.7	131.0	137.1	140.5	142.7
Ovalene series									
C36-C32	60.1	60.3	84.7	102.8	118.6	131.6	138.0	141.7	144.0

Table 3b. Increments

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C40-C38	14.4	14.6	29.7	37.3	43.0	46.8	48.1	48.6	48.7
C42-C40	16.0	16.2	31.9	39.1	44.1	47.4	48.5	48.8	48.8
C54-C42	118.6	119.7	211.7	259.8	296.4	322.4	333.1	338.2	340.6
C66-C54	118.6	119.7	211.7	259.8	296.4	322.4	333.1	338.2	340.6
C80-C66	135.0	136.4	244.4	299.5	341.0	370.1	381.8	387.1	389.6
C96-C80	151.4	153.0	277.0	339.3	385.6	417.7	430.5	436.1	438.5

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C30H14	572.0	574.3	816.9	1042.1	1328.8	1699.2	1982.0	2209.2	2398.6
C34H16	652.9	655.5	934.7	1192.0	1518.6	1939.7	2261.1	2519.3	2734.5
Ovalene series									
C32H14	572.2	574.5	829.6	1066.9	1368.5	1757.5	2054.1	2292.2	2490.5
C36H16	660.9	663.6	955.1	1224.0	1565.2	2005.1	2340.5	2609.8	2834.2
Leading members of series									
C38H16	665.4	668.2	971.6	1253.0	1609.8	2069.0	2418.7	2699.2	2932.7
C40H16	672.2	675.1	990.0	1282.7	1653.9	2131.4	2494.8	2786.0	3028.4
C42H16	672.4	675.4	1002.8	1307.5	1693.6	2189.8	2566.9	2869.0	3120.3
C54H18	778.6	782.4	1195.0	1579.4	2055.1	2687.2	3158.7	3535.8	3849.0
C66H20	903.2	907.6	1405.4	1869.5	2454.9	3202.9	3768.8	4220.9	4595.9
C80H22	1033.8	1039.1	1634.8	2190.9	2891.0	3783.7	4458.0	4995.8	5441.8
C96H24	1170.4	1176.7	1883.3	2543.6	3373.5	4429.7	5226.2	5860.8	6386.4

Table 4a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C34-C30	80.9	81.3	117.8	149.9	189.7	240.5	279.1	310.1	335.9
Ovalene series									
C36-C32	88.7	89.1	125.5	157.1	196.7	247.6	286.4	317.6	343.7

Table 4b. Increments

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C40-C38	6.9	6.9	18.4	29.8	44.1	62.4	76.1	86.9	95.8
C42-C40	.1	.2	12.8	24.8	39.7	58.3	72.1	83.0	91.9
C54-C42	106.3	107.0	192.2	271.9	371.5	497.4	591.8	666.8	728.7
C66-C54	124.5	125.3	210.4	290.1	389.7	515.7	610.1	685.0	747.0
C80-C66	130.6	131.4	229.4	321.4	436.1	580.8	689.1	775.0	845.8
C96-C80	136.7	137.6	248.5	352.6	482.5	646.0	768.2	864.9	944.7

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
Naphthocoronene series									
C30H14	393.5	393.3	379.0	372.1	369.5	374.8	382.0	385.7	383.4
C34H16	437.8	437.6	422.7	415.7	413.4	420.1	428.8	433.3	431.1
Ovalene series									
C32H14	414.9	414.7	400.7	394.3	392.1	397.5	404.2	406.7	402.5
C36H16	457.4	457.2	442.5	435.7	433.7	440.6	449.1	453.0	449.5
Leading members of series									
C38H16	476.6	476.4	461.9	455.8	454.8	462.8	471.5	474.9	470.2
C40H16	497.9	497.7	483.0	477.1	476.0	483.7	491.6	493.7	487.0
C42H16	519.2	519.0	504.7	499.3	498.6	506.4	513.8	514.7	506.2
C54H18	635.8	635.6	621.4	617.5	619.1	629.5	637.2	635.3	620.7
C66H20	752.4	752.1	738.0	735.7	739.5	752.5	760.6	755.9	735.2
C80H22	881.1	880.8	867.3	867.2	873.9	889.8	897.7	889.3	860.6
C96H24	1022.1	1021.8	1009.3	1012.0	1022.1	1041.3	1048.7	1035.2	996.9

Table 5a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C34-C30	44.3	44.3	43.7	43.6	43.9	45.3	46.7	47.6	47.7
Ovalene series									
C36-C32	42.5	42.5	41.7	41.4	41.6	43.1	44.9	46.3	47.0

Table 5b. Increments

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C40-C38	21.2	21.2	21.2	21.2	21.2	20.9	20.1	18.8	16.9
C42-C40	21.4	21.4	21.7	22.2	22.6	22.7	22.2	21.0	19.1
C54-C42	116.6	116.5	116.7	118.2	120.4	123.1	123.4	120.6	114.5
C66-C54	116.6	116.5	116.7	118.2	120.4	123.1	123.4	120.6	114.5
C80-C66	128.8	128.7	129.3	131.5	134.3	137.3	137.2	133.3	125.4
C96-C80	141.0	140.9	142.0	144.8	148.2	151.5	150.9	146.0	136.3

at 298.15 K in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C30H14	547.0	548.0	655.6	767.6	937.9	1221.2	1502.2	1783.5	2061.0
C34H16	613.0	614.1	736.5	863.5	1056.1	1376.3	1693.7	2011.3	2324.6
Ovalene series									
C32H14	571.8	572.7	682.6	796.6	969.7	1257.6	1543.2	1829.3	2112.1
C36H16	633.6	634.7	757.8	885.3	1078.6	1399.9	1718.3	2037.1	2351.7
Leading members of series									
C38H16	655.0	656.1	780.6	909.3	1104.1	1427.3	1747.4	2067.9	2384.4
C40H16	677.6	678.7	804.2	933.9	1130.1	1455.7	1778.5	2101.8	2421.5
C42H16	702.3	703.5	831.2	962.9	1161.9	1492.1	1819.5	2147.7	2472.5
C54H18	846.7	848.0	994.6	1144.8	1370.6	1744.3	2114.6	2486.1	2854.8
C66H20	985.7	987.1	1148.9	1313.8	1561.0	1969.0	2373.1	2778.9	3182.2
C80H22	1138.4	1140.0	1318.0	1498.4	1767.8	2211.4	2650.4	3091.9	3531.5
C96H24	1305.0	1306.7	1501.9	1698.6	1991.1	2471.3	2946.4	3425.0	3902.5

Table 6a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C34-C30	66.0	66.2	80.9	95.9	118.3	155.1	191.5	227.8	263.6
Ovalene series									
C36-C32	61.9	62.0	75.2	88.7	108.9	142.3	175.1	207.7	239.6

Table 6b. Increments

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C40-C38	22.6	22.6	23.6	24.6	26.0	28.4	31.0	33.9	37.1
C42-C40	24.7	24.8	27.0	29.0	31.8	36.4	41.0	45.9	51.0
C54-C42	144.4	144.6	153.4	161.8	168.7	181.8	195.1	208.5	222.3
C66-C54	138.9	139.1	154.3	169.1	190.4	224.7	258.5	292.8	327.5
C80-C66	152.7	152.9	159.1	184.6	206.8	242.3	277.3	312.9	349.2
C96-C80	166.6	166.7	183.9	200.2	223.2	259.9	296.1	333.1	371.0

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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
Naphthocoronene series									
C30H14	.0	.7	97.6	232.4	474.6	932.9	1425.3	1934.4	2453.9
C34H16	.0	.8	112.3	266.2	542.1	1063.2	1622.7	2201.3	2791.7
Ovalene series									
C32H14	.0	.7	102.7	244.6	499.4	980.8	1497.1	2030.5	2574.5
C36H16	.0	.8	117.3	278.1	566.3	1110.7	1694.6	2298.0	2913.4
Leading members of series									
C38H16	.0	.8	122.2	290.4	591.8	1160.1	1768.8	2397.2	3037.7
C40H16	.0	.9	126.8	301.8	615.4	1206.3	1838.8	2491.4	3156.2
C42H16	.0	.9	131.9	314.1	640.2	1254.1	1910.7	2587.5	3276.8
C54H18	.0	1.1	166.2	396.1	806.3	1575.9	2396.9	3241.6	4100.6
C66H20	.0	1.3	200.6	478.1	972.4	1897.8	2883.0	3895.6	4924.4
C80H22	.0	1.6	240.1	572.6	1163.8	2268.1	3441.9	4646.7	5869.8
C96H24	.0	1.9	284.9	679.6	1380.5	2686.9	4073.3	5494.9	6936.7

Table 7a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C34-C30	.0	.1	14.7	33.8	67.5	130.3	197.5	266.9	337.8
Ovalene series									
C36-C32	.0	.1	14.6	33.5	66.9	129.9	197.5	267.5	338.9

Table 7b. Increments

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C40-C38	.0	.0	4.6	11.4	23.6	46.2	70.0	94.2	118.5
C42-C40	.0	.0	5.1	12.2	24.8	47.9	71.9	96.2	120.6
C54-C42	.0	.2	34.4	82.0	166.1	321.8	486.2	654.0	823.8
C66-C54	.0	.2	34.4	82.0	166.1	321.8	486.2	654.0	823.8
C80-C66	.0	.3	39.5	94.5	191.4	370.3	558.8	751.1	945.4
C96-C80	.0	.3	44.7	107.0	216.6	418.8	631.5	848.1	1066.9

relative to the elements at 298.15 K in kJ/mol

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C30H14	393.5	394.2	491.1	625.9	868.1	1325.4	1818.8	2327.9	2847.4
C34H16	437.8	438.6	550.2	704.0	979.9	1501.1	2060.6	2639.1	3229.5
Ovalene series									
C32H14	414.9	415.6	517.6	659.5	914.3	1395.7	1912.0	2445.4	2989.4
C36H16	457.4	458.2	574.7	735.4	1023.7	1563.1	2152.0	2755.4	3370.8
Leading members of series									
C38H16	476.6	477.5	598.8	767.0	1068.5	1635.7	2245.4	2873.8	3514.3
C40H16	497.9	498.7	624.7	799.7	1113.3	1704.1	2336.7	2989.2	3654.0
C42H16	519.2	520.1	651.1	833.3	1159.5	1773.3	2429.9	3106.8	3796.0
C54H18	635.8	636.9	802.0	1031.9	1442.1	2211.7	3032.7	3877.4	4736.4
C66H20	752.4	753.7	952.9	1230.4	1724.8	2650.1	3635.4	4648.0	5676.8
C80H22	881.1	882.7	1121.3	1453.7	2045.0	3149.2	4323.0	5527.9	6750.9
C96H24	1022.1	1024.0	1307.0	1701.7	2402.6	3703.0	5095.4	6517.0	7958.8

Table 8a. Increments per C4H2

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C34-C30	44.3	44.4	59.0	78.2	111.8	174.6	241.8	311.3	382.1
Ovalene series									
C36-C32	42.5	42.6	57.1	76.0	109.4	172.4	240.0	310.0	381.4

Table 8b. Increments

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C40-C38	21.2	21.3	25.9	32.7	44.8	67.4	91.2	115.4	139.7
C42-C40	21.4	21.4	26.4	33.6	46.2	69.2	93.2	117.6	142.0
C54-C42	116.6	116.8	150.9	198.6	282.7	433.4	602.7	770.6	940.4
C66-C54	116.6	116.8	150.9	198.6	282.7	433.4	602.7	770.6	940.4
C80-C66	128.8	129.0	168.3	223.3	320.1	493.1	687.6	879.9	1074.1
C96-C80	141.0	141.2	185.7	248.0	357.6	553.8	772.4	989.1	1207.8

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

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocronene series									
C30H14									
1.	.6640	.6639	.6547	.6446	.6319	.6175	.6084	.6022	.5978
2.	.3320	.3320	.3274	.3223	.3159	.3087	.3042	.3011	.2989
3.	.0041	.0041	.0179	.0331	.0522	.0738	.0874	.0967	.1033
C34H16									
1.	.0760	.0752	.0352	.0235	.0166	.0124	.0107	.0099	.0095
2.	.0760	.0752	.0352	.0235	.0166	.0124	.0107	.0099	.0095
3.	.7853	.7857	.7197	.6263	.5320	.4492	.4061	.3798	.3620
4.	.0037	.0038	.0077	.0097	.0110	.0118	.0123	.0127	.0131
5.	.0037	.0038	.0077	.0097	.0110	.0118	.0123	.0127	.0131
6.	.0037	.0038	.0077	.0097	.0110	.0118	.0123	.0127	.0131
7.	.0019	.0019	.0038	.0048	.0055	.0059	.0062	.0064	.0065
8.	.0000	.0000	.0004	.0010	.0018	.0028	.0035	.0041	.0045
9.	.0001	.0001	.0008	.0020	.0036	.0057	.0071	.0082	.0090
11.	.0037	.0038	.0077	.0097	.0110	.0118	.0123	.0127	.0131
12.	.0000	.0000	.0001	.0004	.0012	.0027	.0041	.0052	.0063
14.	.0037	.0038	.0077	.0097	.0110	.0118	.0123	.0127	.0131
15.	.0192	.0196	.0786	.1288	.1758	.2147	.2335	.2439	.2503
16.	.0001	.0001	.0008	.0020	.0036	.0057	.0071	.0082	.0090
17.	.0192	.0196	.0786	.1288	.1758	.2147	.2335	.2439	.2503
18.	.0000	.0000	.0004	.0010	.0018	.0028	.0035	.0041	.0045
19.	.0037	.0038	.0077	.0097	.0110	.0118	.0123	.0127	.0131
Ovalene series									
C32H14									
ovalene	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C36H16									
1.	.1714	.1704	.1081	.0843	.0683	.0574	.0526	.0500	.0485
2.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
3.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
4.	.0857	.0852	.0940	.0422	.0342	.0287	.0263	.0250	.0243
5.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
6.	.4427	.4450	.5522	.5621	.5485	.5207	.4979	.4795	.4641
7.	.0021	.0021	.0059	.0087	.0113	.0137	.0151	.0161	.0168
8.	.0021	.0021	.0059	.0087	.0113	.0137	.0151	.0161	.0168
9.	.0021	.0021	.0059	.0087	.0113	.0137	.0151	.0161	.0168
10.	.0021	.0021	.0059	.0087	.0113	.0137	.0151	.0161	.0168
11.	.1714	.1704	.1081	.0843	.0683	.0574	.0526	.0500	.0485
12.	.0857	.0852	.0940	.0422	.0342	.0287	.0263	.0250	.0243
13.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
14.	.0001	.0001	.0008	.0020	.0036	.0057	.0071	.0082	.0090
15.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
16.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
17.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
18.	.0042	.0043	.0118	.0173	.0226	.0274	.0302	.0321	.0336
19.	.0001	.0001	.0013	.0036	.0075	.0131	.0174	.0206	.0232
20.	.0010	.0011	.0030	.0043	.0056	.0069	.0076	.0080	.0084

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C38H16									
1. circobiphenyl	.0652	.0651	.0604	.0557	.0504	.0451	.0422	.0403	.0390
2. naphtho(2,1,8-uv)ovalene	.2607	.2606	.2416	.2227	.2016	.1806	.1687	.1612	.1560
3. naphtho(8,1,2-abc)ovalene	.0064	.0065	.0264	.0458	.0666	.0863	.0970	.1035	.1079
4. dibenzo(bc,uv)ovalene	.2607	.2606	.2416	.2227	.2016	.1806	.1687	.1612	.1560
5. dibenzo(hi,uv)ovalene	.2607	.2606	.2416	.2227	.2016	.1806	.1687	.1612	.1560
6. naphtho(2,1,8-bcd)ovalene	.0064	.0065	.0264	.0458	.0666	.0863	.0970	.1035	.1079
7. dibenzo(hi,st)ovalene	.1304	.1303	.1208	.1113	.1008	.0903	.0844	.0806	.0780
8. dibenzo(bc,st)ovalene	.0064	.0065	.0264	.0458	.0666	.0863	.0970	.1035	.1079
9. dibenzo(bc,ef)ovalene	.0032	.0033	.0132	.0229	.0333	.0432	.0485	.0518	.0539
10. dibenzo(bc,mn)ovalene	.0001	.0001	.0014	.0047	.0110	.0206	.0279	.0332	.0373
C40H16									
1. benzo(bc)naphtho(2,1,8,7-stuv)ovalene	.6640	.6639	.6547	.6446	.6319	.6175	.6084	.6022	.5978
2. circum(26)phenanthrene	.3320	.3320	.3274	.3223	.3159	.3087	.3042	.3011	.2989
3. circum(26)anthracene	.0041	.0041	.0179	.0331	.0522	.0738	.0874	.0967	.1033
C42H16	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
circumpyrene									
C54H18	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
circumcoronene									
C66H20	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
circumovalene									
C80H22	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
2-circumpyrene									
C96H24	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
2-circumcoronene									

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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
Naphthocoronene series									
C3CH14									
1. naphtho(8,1-abc)coronene	359.8	362.1	593.9	739.4	861.1	958.1	1004.5	1030.4	1046.3
2. dibenzo(bc,ef)coronene	359.8	362.1	593.9	739.4	861.1	958.1	1004.5	1030.4	1046.3
3. dibenzo(bc,k1)coronene	359.8	362.1	593.9	739.4	861.1	958.1	1004.5	1030.4	1046.3
C34H16									
1. dibenzo(cd,pq)bisanthene	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
2. dibenzo(ef,pq)bisanthene	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
3.	408.2	410.8	673.9	839.2	977.6	1087.9	1140.8	1170.3	1188.3
4.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
5.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
6.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
7.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
8.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
9.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
11.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
12.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
14.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
15.	408.2	410.8	673.9	839.2	977.6	1087.9	1140.8	1170.3	1188.3
16.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
17.	408.2	410.8	673.9	839.2	977.6	1087.9	1140.8	1170.3	1188.3
18.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
19.	412.6	415.1	675.2	840.2	978.9	1089.8	1143.1	1172.8	1191.1
Ovalene series									
C32H14									
ovalene	376.2	378.7	626.5	779.1	905.8	1005.8	1053.2	1079.4	1095.2
C36H16									
1. benzo(cd)dinaphtho(2,1,8,7-fghi:2',1',8'-qrs)anthanth	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
2. pyreno(3,4,5-abc)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
3. benzo(a)ovalene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
4. dinaphtho(8,12-abc:2',1',8'-efg)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
5. dinaphtho(8,1,2-abc:8',1',2'-ghi)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
6. dinaphtho(8,1,2-abc:2',1',8'-nop)coronene	424.7	427.5	706.5	878.9	1022.2	1135.6	1189.4	1219.2	1237.3
7. dinaphtho(8,1,2-abc:2',1',8'-klm)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
8. benzo(d)ovalene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
9. dinaphtho(8,1,2-abc:8',1',2'-jkl)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
10. dinaphtho(8,1,2-abc:2',1',8'-hij)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
11. dibenzo(ef,hi)naphtho(8,1,2-abc)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
12. tetrabenzo(bc,ef,hi,k1)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
13. dibenzo(k1,no)naphtho(8,1,2-abc)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
14. pyreno(4,9,2-abc)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
15. benzo(op)dinaphtho(8,1,2-bcd:2',1',8',7'-fghi)anthanthr	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
16. dibenzo(ef,no)naphtho(8,1,2-abc)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
17. dibenzo(hi,kl)naphtho(8,1,2-abc)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
18. anthra(1,9,8-abcd)benzo(hi)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
19. dibenzo(ijk,tuv)naphtho(8,1,2-efg)beropvrene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0

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
20. tetrabenzo(bc,ef,k,l,no)coronene	429.1	431.8	707.8	880.0	1023.6	1137.5	1191.7	1221.8	1240.0
Leading members of series									
C38H16									
1. circobiphenyl	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
2. naphtho(2,1,8-uva)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
3. naphtho(8,1,2-abc)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
4. dibenzo(bc,uv)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
5. dibenzo(hi,uv)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
6. naphtho(2,1,8-bcd)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
7. dibenzo(hi,st)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
8. dibenzo(bc,st)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
9. dibenzo(bc,ef)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
10. dibenzo(bc,mn)ovalene	445.5	448.5	740.4	919.7	1068.2	1185.2	1240.4	1270.7	1289.0
C40H16									
1. benzo(bc)naphtho(2,1,8,7-stuv)ovalene	462.0	465.1	773.0	959.5	1112.8	1232.8	1289.0	1319.7	1337.9
2. circum(26)phenanthrene	462.0	465.1	773.0	959.5	1112.8	1232.8	1289.0	1319.7	1337.9
3. circum(26)anthracene	462.0	465.1	773.0	959.5	1112.8	1232.8	1289.0	1319.7	1337.9
C42H16									
circumpyrene	478.4	481.8	805.6	999.2	1157.5	1280.5	1337.7	1368.6	1386.9
C54H18									
circumcoronene	597.0	601.5	1017.4	1259.0	1453.8	1602.9	1670.8	1706.8	1727.5
C66H20									
circumovalene	715.5	721.2	1229.1	1518.8	1750.2	1925.3	2004.0	2045.0	2068.2
C80H22									
2-circumpyrene	850.6	857.6	1473.5	1818.3	2091.2	2295.3	2385.8	2432.1	2457.7
C96H24									
2-circumcoronene	1002.0	1010.6	1750.5	2157.6	2476.8	2713.1	2816.2	2868.2	2896.3

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

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C30H14									
1. naphtho(8,1-abc)coronene	568.5	570.7	813.0	1038.0	1324.5	1694.7	1977.4	2204.6	2394.0
2. dibenzo(bc,ef)coronene	562.7	565.0	807.3	1032.3	1318.8	1689.0	1971.7	2198.9	2388.3
3. dibenzo(bc,k1)coronene	557.0	559.2	801.5	1026.5	1313.0	1683.2	1965.9	2193.1	2382.5
C34H16									
1. dibenzo(cd,pq)bisanthene	617.3	619.9	896.0	1151.7	1477.4	1898.3	2219.9	2478.5	2694.1
2. dibenzo(ef,pq)bisanthene	617.3	619.9	896.0	1151.7	1477.4	1898.3	2219.9	2478.5	2694.1
3. benzo(a)ovalene	651.6	654.1	929.0	1184.4	1509.6	1929.9	2250.9	2508.9	2724.0
4. dinaphtho(8,12-abc;2',1',8'-efg)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
5. dinaphtho(8,1,2-abc;8',1',2'-ghi)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
6. dinaphtho(8,1,2-abc;2',1',8'-nop)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
7. dinaphtho(8,1,2-abc;2',1',8'-klm)coronene	617.3	619.9	896.0	1151.7	1477.4	1898.3	2219.9	2478.5	2694.1
8. dinaphtho(8,1,2-abc;8',1',2'-jkl)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
9. dinaphtho(8,1,2-abc;2',1',8'-hij)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
10. dinaphtho(8,1,2-abc;2',1',8'-hij)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
11. dinaphtho(8,1,2-abc;2',1',8'-nop)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
12. tetraabenzobenzene	651.6	654.1	929.0	1184.4	1509.6	1929.9	2250.9	2508.9	2724.0
13. dibenzo(k1,no)naphtho(8,1,2-abc)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
14. benzo(op)dinaphtho(8,1,2-bcd;2',1',8',7'-fghi)anthanthr	651.6	654.1	929.0	1184.4	1509.6	1929.9	2250.9	2508.9	2724.0
15. benzo(op)dinaphtho(8,1,2-abc)coronene	617.3	619.9	896.0	1151.7	1477.4	1898.3	2219.9	2478.5	2694.1
16. dibenzo(hi,kl)naphtho(8,1,2-abc)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
17. anthra(1,9,8-abcd)benzo(hi)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
18. anthra(1,9,8-abcd)benzo(hi)coronene	623.1	625.7	901.8	1157.5	1483.1	1904.1	2225.7	2484.3	2699.8
Ovalene series									
C32H14									
1. ovalene	572.2	574.5	829.6	1066.9	1368.5	1757.5	2054.1	2292.2	2490.5
C36H16									
1. benzo(cd)dinaphtho(2,1,8,7-fghi;2',1',8'-qrs)anthanthr	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
2. pyreno(3,4,5-abc)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
3. benzo(a)ovalene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
4. dinaphtho(8,12-abc;2',1',8'-efg)coronene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
5. dinaphtho(8,1,2-abc;8',1',2'-ghi)coronene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
6. dinaphtho(8,1,2-abc;2',1',8'-nop)coronene	661.0	663.7	951.4	1219.0	1559.3	1998.4	2333.3	2602.3	2826.3
7. dinaphtho(8,1,2-abc;2',1',8'-klm)coronene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
8. benzo(d)ovalene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
9. dinaphtho(8,1,2-abc;8',1',2'-jkl)coronene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
10. dinaphtho(8,1,2-abc;2',1',8'-hij)coronene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
11. dinaphtho(8,1,2-abc)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
12. tetraabenzobenzene	632.5	635.2	924.1	1192.1	1532.9	1972.6	2308.1	2577.6	2802.1
13. dibenzo(k1,no)naphtho(8,1,2-abc)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
14. pyreno(4,3,2-abc)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
15. benzo(op)dinaphtho(8,1,2-bcd;2',1',8',7'-fghi)anthanthr	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
16. dibenzo(ef,no)naphtho(8,1,2-abc)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
17. dibenzo(hi,kl)naphtho(8,1,2-abc)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8
18. anthra(1,9,8-abcd)benzo(hi)coronene	638.3	641.0	929.9	1197.9	1538.6	1978.4	2313.9	2583.3	2807.8

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

T/K	298	300	500	700	1000	1500	2000	2500	3000
Leading members of series									
C3H16									
1. circobiphenyl	642.0	644.7	946.5	1226.7	1582.6	2041.2	2390.5	2670.9	2904.3
2. naphtho(2,1,8-uv)ovalene	653.5	656.3	958.0	1238.3	1594.1	2052.7	2402.1	2682.4	2915.8
3. naphtho(8,1,2-abc)ovalene	653.5	656.3	958.0	1238.3	1594.1	2052.7	2402.1	2682.4	2915.8
4. dibenzo(bc,uv)ovalene	653.5	656.3	958.0	1238.3	1594.1	2052.7	2402.1	2682.4	2915.8
5. dibenzo(hi,uv)ovalene	653.5	656.3	958.0	1238.3	1594.1	2052.7	2402.1	2682.4	2915.8
6. naphtho(2,1,8-bcd)ovalene	647.7	650.5	952.3	1232.5	1588.4	2046.9	2396.3	2676.6	2910.1
7. dibenzo(hi,st)ovalene	653.5	656.3	958.0	1238.3	1594.1	2052.7	2402.1	2682.4	2915.8
8. dibenzo(bc,st)ovalene	647.7	650.5	952.3	1232.5	1588.4	2046.9	2396.3	2676.6	2910.1
9. dibenzo(bc,ef)ovalene	647.7	650.5	952.3	1232.5	1588.4	2046.9	2396.3	2676.6	2910.1
10. dibenzo(bc,mn)ovalene	647.7	650.5	952.3	1232.5	1588.4	2046.9	2396.3	2676.6	2910.1
C4OH16									
1. benzo(bc)naphtho(2,1,8,7-stuv)ovalene	668.7	671.6	986.2	1278.7	1649.6	2127.0	2490.2	2781.5	3023.8
2. circum(26)phenanthrene	662.9	665.8	980.4	1272.9	1643.9	2121.2	2484.5	2775.7	3018.1
3. circum(26)anthracene	657.2	660.1	974.7	1267.1	1638.1	2115.5	2478.7	2770.0	3012.3
C42H16									
circumpyrene	672.4	675.4	1002.8	1307.5	1693.6	2189.8	2566.9	2869.0	3120.3
C54H18									
circumcoronene	778.6	782.4	1195.0	1579.4	2065.1	2687.2	3158.7	3535.8	3849.0
C66H20									
circumovalene	903.2	907.6	1405.4	1869.5	2454.9	3202.9	3768.8	4230.9	4595.9
C80H22									
2-circumpyrene	1033.8	1039.1	1634.8	2190.9	2891.0	3783.7	4458.0	4995.8	5441.8
C96H24									
2-circumcoronene	1170.4	1176.7	1883.3	2543.6	3373.5	4429.7	5226.2	5860.8	6386.4

THERMODYNAMIC PROPERTIES OF POLYCYCLIC AROMATIC HYDROCARBONS

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

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C30H14									
1. raphtho(8,1-abc)coronene	393.5	393.3	378.9	371.8	369.0	374.1	381.2	384.8	382.4
2. cibenzo(bc,ef)coronene	393.5	393.3	378.9	371.8	369.0	374.1	381.2	384.8	382.4
3. cibenzo(bc,kl)coronene	402.7	402.5	388.1	381.0	378.2	383.3	390.4	394.0	391.6
C34H16									
1. cibenzo(cd,pq)bisanthene	433.6	433.4	417.3	409.3	406.3	412.8	421.9	427.2	425.9
2. cibenzo(ef,pq)bisanthene	433.6	433.4	417.3	409.3	406.3	412.8	421.9	427.2	425.9
3.	438.0	437.8	421.2	413.1	409.7	415.4	423.4	427.5	424.9
4.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
5.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
6.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
7.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
8.	452.0	451.8	435.7	427.7	424.7	431.2	440.3	445.6	444.3
9.	442.0	441.8	426.5	418.5	415.5	422.0	431.1	436.4	435.1
10.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
11.	461.2	461.0	444.9	436.9	433.9	440.4	449.5	454.8	453.5
12.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
13.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
14.	447.2	447.0	430.4	422.3	418.9	424.6	432.6	437.7	434.1
15.	447.2	447.0	430.4	422.3	418.9	424.6	432.6	437.7	434.1
16.	452.0	451.8	435.7	427.7	424.7	431.2	440.3	445.6	444.3
17.	447.2	447.0	430.4	422.3	418.9	424.6	432.6	437.7	434.1
18.	452.0	451.8	435.7	427.7	424.7	431.2	440.3	445.6	444.3
19.	442.8	442.6	426.5	418.5	415.5	422.0	431.1	436.4	435.1
Ovalene series									
C32H14									
ovalene	414.9	414.7	400.7	394.3	392.1	397.5	404.2	406.7	402.5
C36H16									
1. benzo(cd)dinaphtho(2,1,8,7-fghi:2',1',8'-qrs)anthanthr	455.0	454.8	439.1	431.8	429.4	436.2	444.9	449.0	445.9
2. pyreno(3,4,5-abc)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
3. benzo(a)ovalene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
4. cinaphtho(8,12-abc:2',1',8'-efg)coronene	455.0	454.8	439.1	431.8	429.4	436.2	444.9	449.0	445.9
5. cinaphtho(8,1,2-abc:8',1',2'-ghi)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
6. cinaphtho(8,1,2-abc:2',1',8'-nop)coronene	459.4	459.2	443.1	435.6	432.8	438.8	446.4	449.4	444.9
7. dinaphtho(8,1,2-abc:2',1',8'-klm)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
8. benzo(d)ovalene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
9. cinaphtho(8,1,2-abc:8',1',2'-jkl)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
10. cinaphtho(8,1,2-abc:2',1',8'-hij)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
11. dibenzo(ef,hi)naphtho(8,1,2-abc)coronene	455.0	454.8	439.1	431.8	429.4	436.2	444.9	449.0	445.9
12. tetrabenzo(bc,ef,hi,kl)coronene	455.0	454.8	439.1	431.8	429.4	436.2	444.9	449.0	445.9
13. dibenzo(kl,no)naphtho(8,1,2-abc)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
14. pyreno(4,3,2-abc)coronene	473.4	473.2	457.5	450.2	447.8	454.6	463.3	467.5	464.4
15. benzo(op)dinaphtho(8,1,2-bcd:2',1',8'-fghi)anthanthr	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
16. dibenzo(ef,no)naphtho(8,1,2-abc)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
17. dibenzo(hi,kl)naphtho(8,1,2-abc)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
18. anthra(1,9-abcd)benzo(hi)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1

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T/K	298	300	500	700	1000	1500	2000	2500	3000
20. tetrabenzo(bc,ef,k1,no)coronene	464.2	464.0	448.3	441.0	438.6	445.4	454.1	458.2	455.1
Leading members of series									
C38H16									
1. circobiphenyl	476.4	476.2	461.0	454.3	452.5	459.6	467.9	470.9	466.0
2. naphtho(2,1,8-uva)ovalene	476.4	476.2	461.0	454.3	452.5	459.6	467.9	470.9	466.0
3. naphtho(8,1,2-abc)ovalene	485.6	485.4	470.2	463.5	461.7	468.8	477.1	480.1	475.2
4. cibenzo(bc,uv)ovalene	476.4	476.2	461.0	454.3	452.5	459.6	467.9	470.9	466.0
5. cibenzo(hi,uv)ovalene	476.4	476.2	461.0	454.3	452.5	459.6	467.9	470.9	466.0
6. naphtho(2,1,8-bcd)ovalene	485.6	485.4	470.2	463.5	461.7	468.8	477.1	480.1	475.2
7. dibenzo(hi,st)ovalene	476.4	476.2	461.0	454.3	452.5	459.6	467.9	470.9	466.0
8. dibenzo(bc,st)ovalene	485.6	485.4	470.2	463.5	461.7	468.8	477.1	480.1	475.2
9. dibenzo(bc,ef)ovalene	485.6	485.4	470.2	463.5	461.7	468.8	477.1	480.1	475.2
10. dibenzo(bc,mn)ovalene	494.8	494.6	479.4	472.7	470.9	478.0	486.3	489.3	484.4
C40H16									
1. benzo(bc)naphtho(2,1,8,7-stuv)ovalene	497.8	497.6	482.9	476.8	475.6	483.0	490.8	492.8	486.1
2. circum(26)phenanthrene	497.8	497.6	482.9	476.8	475.6	483.0	490.8	492.8	486.1
3. circum(26)anthracene	507.0	506.8	492.1	486.0	484.8	492.2	500.0	502.0	495.3
C42H16									
circumpyrene	519.2	519.0	504.7	499.3	498.6	506.4	513.8	514.7	506.2
C54H18									
circumcoronene	635.8	635.6	621.4	617.5	619.1	629.5	637.2	635.3	620.7
C66H20									
circumovalene	752.4	752.1	738.0	735.7	739.5	752.5	760.6	755.9	735.2
C80H22									
2-circumpyrene	881.1	880.8	867.3	857.2	873.9	889.8	897.7	889.3	860.6
C96H24									
2-circumcoronene	1022.1	1021.8	1009.3	1012.0	1022.1	1041.3	1048.7	1035.2	996.9

THERMODYNAMIC PROPERTIES OF POLYCYCLIC AROMATIC HYDROCARBONS

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

T/K	298	300	500	700	1000	1500	2000	2500	3000
Naphthocoronene series									
C30H14									
1. naphtho(8,1-abc)coronene	548.0	549.0	657.4	770.2	941.7	1227.2	1510.5	1794.0	2073.9
2. dibenzo(bc,ef)coronene	549.8	550.7	660.2	774.2	947.4	1235.9	1522.0	1808.4	2091.2
3. dibenzo(bc,k1)coronene	560.7	561.7	672.3	787.5	962.4	1253.7	1542.7	1832.0	2117.7
C34H16									
1. dibenzo(cd,pq)bisanthene	619.4	620.6	750.5	885.4	1090.2	1431.1	1769.1	2107.2	2440.9
2. dibenzo(ef,pq)bisanthene	619.4	620.6	750.5	885.4	1090.2	1431.1	1769.1	2107.2	2440.9
3.	613.6	614.7	737.9	866.2	1061.4	1386.3	1708.7	2031.4	2350.0
4.	626.9	628.1	756.8	890.5	1093.6	1431.7	1766.8	2102.0	2432.8
5.	626.9	628.1	756.8	890.5	1093.6	1431.7	1766.8	2102.0	2432.8
6.	626.9	628.1	756.8	890.5	1093.6	1431.7	1766.8	2102.0	2432.8
7.	628.6	629.8	759.7	894.6	1099.4	1440.3	1778.3	2116.4	2450.1
8.	637.8	639.0	768.9	903.8	1108.6	1449.5	1787.6	2125.7	2459.3
9.	636.1	637.3	766.0	899.7	1102.9	1440.9	1776.0	2111.2	2442.0
11.	626.9	628.1	756.8	890.5	1093.6	1431.7	1766.8	2102.0	2432.8
12.	645.3	646.5	775.2	908.9	1112.1	1450.1	1785.2	2120.4	2451.2
14.	626.9	628.1	756.8	890.5	1093.6	1431.7	1766.8	2102.0	2432.8
15.	622.9	623.9	747.1	875.5	1070.6	1395.5	1717.9	2040.6	2359.2
16.	636.1	637.3	766.0	899.7	1102.9	1440.9	1776.0	2111.2	2442.0
17.	622.9	623.9	747.1	875.5	1070.6	1395.5	1717.9	2040.6	2359.2
18.	637.8	639.0	768.9	903.8	1108.6	1449.5	1787.6	2125.7	2459.3
19.	626.9	628.1	756.8	890.5	1093.6	1431.7	1766.8	2102.0	2432.8
Ovalene series									
C32H14									
ovalene	571.8	572.7	682.6	796.6	969.7	1257.6	1543.2	1829.3	2112.1
C36H16									
1. benzo(cd)dinaphthol(2,1,8,7-fghi:2',1',8'-qrs)anthanth	638.0	639.1	767.0	899.7	1100.9	1435.6	1767.3	2099.3	2427.2
2. pyreno(3,4,5-abc)coronene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
3. benzo(a)ovalene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
4. dinaphtho(8,12-abc:2',1',8'-efg)coronene	639.7	640.9	769.9	903.7	1106.7	1444.2	1776.9	2113.7	2444.5
5. dinaphtho(8,1,2-abc:8',1',2'-ghi)coronene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
6. dinaphtho(8,1,2-abc:2',1',8'-nop)coronene	635.7	636.8	760.3	888.7	1083.6	1408.1	1729.9	2052.4	2370.8
7. dinaphtho(8,1,2-abc:2',1',8'-klm)coronene	648.9	650.1	779.1	912.9	1115.9	1453.4	1788.1	2123.0	2453.7
8. benzo(d)ovalene	648.9	650.1	779.1	912.9	1115.9	1453.4	1788.1	2123.0	2453.7
9. dinaphtho(8,1,2-abc:8',1',2'-jkl)coronene	648.9	650.1	779.1	912.9	1115.9	1453.4	1788.1	2123.0	2453.7
10. dinaphtho(8,1,2-abc:2',1',8'-hij)coronene	648.9	650.1	779.1	912.9	1115.9	1453.4	1788.1	2123.0	2453.7
11. dibenzo(ef,hi)naphtho(8,1,2-abc)coronene	638.0	639.1	767.0	899.7	1100.9	1435.6	1767.3	2099.3	2427.2
12. tetrabenzo(bc,ef,hi,kl)coronene	639.7	640.9	769.9	903.7	1106.7	1444.2	1776.9	2113.7	2444.5
13. dibenzo(kl,nc)naphtho(8,1,2-abc)coronene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
14. pyreno(4,3,2-abc)coronene	656.4	657.6	785.4	918.1	1119.3	1454.0	1785.7	2117.7	2445.6
15. benzo(op)dinaphtho(8,1,2-bcd:2',1',8',7'-fghi)anthanthr	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
16. benzo(ef,no)naphtho(8,1,2-abc)coronene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
17. dibenzo(hi,kl)naphtho(8,1,2-abc)coronene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
18. anthra(1,9,8-abc)benzo(hi)coronene	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4
19. dibenzo(iik,ti)lnaphtho(8,1,2-efgh)anthanthr	647.2	648.4	776.2	908.9	1110.1	1444.8	1776.5	2108.5	2436.4

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

T/K	298	300	500	700	1000	1500	2000	2500	3000
20. tetrabenzo(bc,ef,k,l,nc)coronene	650.7	651.8	782.0	917.0	1121.7	1462.1	1799.6	2137.4	2471.0
Leading members of series									
C38H16									
1. circobiphenyl	661.7	662.9	792.3	926.2	1129.0	1466.0	1800.1	2134.7	2465.3
2. naphtho(2,1,8-uv)ovalene	658.3	659.4	786.5	918.1	1117.4	1448.7	1777.0	2105.8	2430.8
3. naphtho(8,1,2-abc)ovalene	667.5	668.6	795.7	927.3	1126.6	1457.9	1786.2	2115.1	2440.0
4. dibenzo(bc,uv)ovalene	658.3	659.4	786.5	918.1	1117.4	1448.7	1777.0	2105.8	2430.8
5. dibenzo(hi,uv)ovalene	657.5	658.6	786.5	918.1	1117.4	1448.7	1777.0	2105.8	2430.8
6. naphtho(2,1,8-bcd)ovalene	660.0	661.2	789.4	922.1	1123.2	1457.3	1788.6	2120.3	2448.1
7. dibenzo(hi,st)ovalene	667.5	668.6	795.7	927.3	1126.6	1457.9	1786.2	2115.1	2440.0
8. dibenzo(bc,st)ovalene	669.2	670.4	798.6	931.3	1132.4	1466.5	1797.8	2129.5	2457.3
10. dibenzo(bc,mn)ovalene	678.4	679.6	807.8	940.5	1141.6	1475.7	1807.0	2138.7	2466.5
C40H16									
1. benzo(bc)naphtho(2,1,8,7-stuv)ovalene	678.6	679.7	806.0	936.5	1133.9	1461.8	1786.7	2112.4	2434.4
2. circum(26)phenanthrene	680.3	681.5	808.8	940.5	1139.7	1470.4	1798.3	2126.8	2451.6
3. circum(26)anthracene	691.2	692.4	820.9	953.7	1154.7	1488.3	1819.0	2150.4	2478.1
C42H16									
circumpyrene	702.3	703.5	831.2	962.9	1151.9	1492.1	1819.5	2147.7	2472.5
C54H18									
circumcoronene	846.7	848.0	994.6	1144.8	1370.6	1744.3	2114.6	2486.1	2854.8
C66H20									
circumovalene	985.7	987.1	1148.9	1313.8	1561.0	1969.0	2373.1	2778.9	3182.2
C80H22									
2-circumpyrene	1138.4	1140.0	1318.0	1498.4	1767.8	2211.4	2650.4	3091.9	3531.5
C96H24									
2-circumcoronene	1305.0	1306.7	1501.9	1698.6	1991.1	2471.3	2946.4	3425.0	3902.5

Table 14. Parameters in kJ/mol for calculating Gibbs energies of formation of the most condensed benzenoid polycyclic aromatic hydrocarbons using equation 4

T/K	298.15	300	500	700	1000	1500	2000	2500	3000
a	-128.600	-129.100	-158.300	-187.200	-228.100	-296.900	-363.400	-427.200	-490.500
b	5.550	5.542	5.125	4.575	3.650	1.942	-.242	-1.342	-2.808
c	37.533	37.658	48.675	60.275	77.867	107.575	136.942	165.875	194.275

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9. Nomenclature

C_p°	= standard heat capacity at constant pressure of isomer i , $J K^{-1} mol^{-1}$
$C_p^\circ(I)$	= standard heat capacity at constant pressure of isomer group I, $J K^{-1} mol^{-1}$
$\Delta_f G_i^\circ$	= 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, $kJ mol^{-1}$
$H^\circ(I,T) - H^\circ(I,298.15 K)$	= standard enthalpy for isomer groups relative to isomer groups at 298.15 K, $kJ mol^{-1}$
$H^\circ(I,T) - H^\circ(I,298.15 K) + \Delta_f H^\circ(I,298.15 K)$	= standard enthalpy for isomer groups relative to elements at 298.15 K, $kJ mol^{-1}$
$\Delta_f H_i^\circ$	= 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 , $J K^{-1} mol^{-1}$
$S^\circ(I)$	= 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

- R. A. Alberty and A. K. Reif, *J. Phys. Chem. Ref. Data* **17**, 241 (1988).
- R. A. Alberty, M. B. Chung, and A. K. Reif, *J. Phys. Chem. Ref. Data* **18**, 77 (1989).
- J. R. Dias, *Accounts Chem. Res.* **18**, 241 (1985).
- J. R. Dias, *J. Macromol. Sci. Chem.* **22**(3), 335 (1985).
- J. R. Dias, *J. Mol. Struct. (Theochem.)* **137**, 9 (1986).
- J. R. Dias, *J. Mol. Struct. (Theochem.)* **149**, 213 (1987).
- J. R. Dias, "Part A: Benzenoid Hydrocarbons," in *Handbook of Polycyclic Hydrocarbons* (Elsevier, Amsterdam, 1987).
- J. R. Dias, "Part B: Polycyclic Isomers and Heteroatom Analogs of Benzenoid Hydrocarbons," in Elsevier, Amsterdam, 1988.
- J. V. Knop, W. Müller, K. Szmanski, and N. Trinajstić, "Computer Generation of Certain Classes of Molecules"; SKTH/Kemija u industriji, Zagreb, 1985.
- R. A. Alberty and C. A. Gehrig, *J. Phys. Chem. Ref. Data* **13**, 11 (1984).
- R. A. Alberty, *J. Phys. Chem. Ref. Data* **14**, 177 (1985).
- R. A. Alberty and C. A. Gehrig, *J. Phys. Chem. Ref. Data* **14**, 803 (1985).
- R. A. Alberty and T. M. Bloomstein, *J. Phys. Chem. Ref. Data* **14**, 8 (1985).
- R. A. Alberty and Y. S. Ha, *J. Phys. Chem. Ref. Data* **14**, 1107 (1985).
- R. A. Alberty and E. Burmenko, *J. Phys. & Chem. Ref. Data* **15**, 13 (1986).
- R. A. Alberty, E. Burmenko, and M. Chung, *J. Phys. Chem. Ref. Data* **16**, 193 (1987).
- R. A. Alberty, M. B. Chung, and T. M. Flood, *J. Phys. Chem. Ref. Data* **16**, 391 (1987).
- B. D. Smith, *AIChE J.* **5**, 26 (1959).
- W. R. Smith and R. W. Missen, *Chemical Reaction Equilibrium Analysis: Theory and Algorithms* (Wiley-Interscience, New York, 1982).
- R. A. Alberty, *Ind. Eng. Chem. Fund.* **22**, 318 (1983).
- S. W. Benson, *Thermochemical Kinetics* (Wiley, New York, 1976).
- S. E. Stein, D. M. Golden, and S. W. Benson, *J. Phys. Chem.* **81**, 3 (1977).
- S. E. Stein and A. Fahr, *J. Phys. Chem.* **89**, 3714 (1985).
- B. Nelander and S. J. Sunner, *Chem. Phys.* **44**, 2476 (1966).
- E. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, M. Bailey, K. L. Chruney, and R. L. Nuttall, "The NSB tables of chemical thermodynamic properties." *J. Phys. Chem. Ref. Data* **11**, Suppl. No. (1982).
- M. W. Chase, C. A. Davies, J. R. Downey, D. J. Frurip, R. A. McDonald and A. N. Syverud, *JANAF Thermochemical Tables*, Third Ed., *J. Phys. Chem. Ref. Data* **14**, Suppl. No. 1 (1985).
- E. R. Cohen and B. N. Taylor, *The 1986 Adjustment of the Fundamental Physical Constants*, CODATA Bulletin, No. 63, 1986.
- TRC Thermodynamic Tables, Hydrocarbons, Vols. 7 and 8, Thermodynamics Research Center, The Texas A & M University System, College Station, Texas, 1986.
- J. B. Pedley, R. D. Naylor, and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed. (Chapman and Hall, New York, 1986).
- I. Mills et al., *Quantities, Units and Symbols in Physical Chemistry* (Blackwell Scientific, Boston (1988)).
- Nomenclature of Organic Chemistry*, edited by J. Rigaudy and S. P. Kliney (Pergamon, New York, 1979).
- O. V. Dorofeeva and L. V. Gurvich, *Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons in the Gaseous Phase* (Institute for High Temperatures, USSR Academy of Sciences, Moscow, 1988) (preprint no. 238).
- R. A. Alberty and I. Oppenheim, *J. Chem. Phys.* **89**, 3689 (1988).
- R. A. Alberty, *J. Chem.* **93**, 3299 (1989).

11. Appendix

TABLE A.1. Group additivity values of Stein and Fahr for benzenoid aromatic hydrocarbons.

Group	$\frac{\Delta H^\circ_{298}}{\text{kJ mol}^{-1}}$	$\frac{S^\circ_{298}}{\text{JK}^{-1} \text{mol}^{-1}}$	$C_p^\circ / \text{J K}^{-1} \text{mol}^{-1}$										
			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