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Densities of Polycyclic Hydrocarbons

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1 Introduction

1.1 Basic Concepts

The mass density of a substance is an intensive quantity defined by:

$$\rho = m / v \quad (1.1)$$

where m is the mass and v is the volume of the sample. Both these quantities are extensive quantities. Other densities often referred to in the literature are the relative density and the molar density. Relative density, also called specific gravity, is:

$$\rho_r = \rho / \rho_0 \quad (1.2)$$

where ρ_0 is the density of a standard substance. It is necessary to specify the conditions of temperature and pressure for the standard substance. The most common reference material is water often at the temperature of its maximum density, 4 °C, at atmospheric pressure. The molar density is defined as

$$\rho_m = 1 / V \quad (1.3)$$

where V is the volume occupied by one mole of the substance. The only densities reported in this volume are the mass densities; relative and molar densities have been converted to mass densities, and all densities have been reported in SI units. If the mass, m , in equation (1.1) has not been corrected for air buoyancy it gives the apparent density in air. The API specific gravity is: $\rho \text{ (API)} = 141.5 / \rho_r - 131.5$, in which ρ_r is $\rho(288.68 \text{ K}) / \rho_0(288.68 \text{ K})$, and the standard substance is water at 288.68 K (60 °F).

The density of a material is a function of temperature and pressure but its value at some standard condition (for example, 293.15 K or 298.15 K at either atmospheric pressure or at the vapor pressure of the compound) often is used to characterize a compound and to ascertain its purity. Accurate density measurements as a function of temperature are important for custody transfer of materials when the volume of the material transferred at a specific temperature is known but contracts specify the mass of material transferred. Engineering applications utilize the density of a substance widely, frequently for the efficient design and safe operation of chemical plants and equipment. The density and the vapor pressure are the most often-quoted properties of a substance, and the properties most often required for prediction of other properties of the substance. In this volume, we do not report the density of gases, but rather the densities of solids as a function of temperature at atmospheric pressure and the densities of liquids either at atmospheric pressure or along the saturation line up to the critical temperature.

The purpose of this compilation is to tabulate the densities of compounds, hence only minimal description of experimental methods used to measure the density of liquids or solids appears. Detailed descriptions of methods for density determination of solids, liquids and gases, along with appropriate density reference standards, appear in a chapter by Davis and Koch in *Physical Methods of Chemistry*, Volume VI, Determination of Thermodynamic Properties [86-ros/bae].

The two principal experimental apparatuses used to determine the density of a liquid are: the pycnometer and the vibrating tube densimeter. The pycnometer method involves measuring the mass of a liquid in a vessel of known volume. The volume of the pycnometer, either at the temperature of measurement or at some reference temperature, is determined using a density standard, usually water or mercury. Using considerable care and a precision analytical balance accurate to $\pm 10^{-5}$ g, it is possible to achieve densities accurate to a few parts in 10^6 with a pycnometer having a volume of 25 cm³ to 50 cm³.

It is common to achieve accuracies of 1 part in 10^5 in using equation (1.1) with pycnometers as small as 5 cm^3 and routine measurements can achieve 1 part in 10^4 . However the main sources of error in assigning density to a particular compound in a particular state arise from factors other than the measurement of mass and volume. See Section 1.4.1

The vibrating tube densimeter relies upon the fact that the frequency f of vibration for a U or V shaped tube depends upon the mass of material in the tube:

$$\rho = A / f^2 + B \quad (1.4)$$

Calibration of the apparatus is necessary; usually water and air or nitrogen are the reference materials. Vibrating tube densimeters designed to operate close to atmospheric pressure can achieve repeatability of parts in 10^6 . If the reciprocal of the frequency is linear in density, accuracies of 1 part in 10^5 are readily achievable.

The principal experimental method used to measure the density of a solid is determination of the mass of liquid displaced by a known mass of solid. It is essential that the solid have no appreciable solubility in the liquid, that all occluded air be removed from the solid and that the density of the displacement fluid be less than that of the solid lest the solid float. Densities of crystalline solids also can be determined from the dimensions of the unit cell. Davis and Koch discuss other methods for measuring the density of liquids and solids such as: hydrostatic weighing of a buoy and flotation methods.

1.2 Scope of the Compilation

Volume IV/8F presents observed values for the densities of hydrocarbons containing two or more rings. These values represent a compilation and evaluation of data from the scientific literature covering approximately the past 100 years. The values presented come from the TRC Source Database. The Thermodynamics Research Center has assembled these data over a period of years and has used them to provide the evaluated density values listed in the TRC Thermodynamic Tables - Hydrocarbons. An additional literature search has been performed immediately before producing this compilation to locate new or missing data and to bring the collection up-to-date. This compilation should include at least 90% of the pertinent data reported in the literature. The usual experimental conditions are in contact with air at one atmosphere below the normal boiling point of the hydrocarbon, and in equilibrium with the vapor phase above the normal boiling point. In the summary tables, temperatures reported on the Kelvin scale have been obtained by adding 273.15 to temperatures originally given on the Celsius scale.

Densities have units of kilograms per cubic meter ($\text{kg}\cdot\text{m}^{-3}$). Values reported in units of grams per milliliter, where the liter is "the volume of one kilogram of water at its temperature of maximum density" convert to $\text{kg}\cdot\text{m}^{-3}$ when multiplied by 999.972 (as defined by the 12th General Conference of the International Committee on Weights and Measure, 1964). Values of specific gravity relative to water at a stated reference temperature become density upon multiplication by the accepted density of water at the reference temperature. Most reported densities for liquids below the boiling point apply to the air-saturated liquid.

Compounds are identified by an IUPAC approved name [93-ano-1], the empirical molecular formula, and the Chemical Abstracts Service Registry Number. A summary table is available for each compound which includes the reported temperature and density values, an assigned uncertainty for the density, the difference between the observed and smoothed density values and an index key to the source of the data. A complete list of references, identified by the index keys, appears at the end of the volume.

Where appropriate, tables of smoothed, recommended values are given at integral multiples of 10 K over the experimental range of temperatures. Values at 293.15 K and 298.15 K are included when they are in the range of the original data set. The recommended values also have assigned uncertainties.

1.3 Description of Data Tables

Data for a particular compound are selected, evaluated and smoothed in one of four ways, depending upon the number and accuracy of the reported values and upon their distribution over the temperature range.

Case 1. When the data set consists of at least four acceptable, effectively distinct values (see section 1.5.3), the densities in selected subsets are fit to a function of temperature using the least squares criterion. A summary table for the selected set gives the densities, their estimated uncertainties, the deviations between observed and calculated values, an index key to the list of references and a plotting symbol. If sufficient space remains, some data outside the selected set also are included in the summary table along with reference keys to any remaining data. A plot of the deviations between observed and calculated values is shown for the selected subset. Error bars indicate the size of the estimated uncertainties for the data. Distinct plotting symbols identify the five data sources that have the smallest average estimated uncertainties. A single symbol represents all remaining data in the selected set. A table consisting of smoothed, recommended values (calculated from the fitted functions) is also given. Estimated uncertainties are given for the recommended values which also appear as a continuous line on the deviation plot. Densities of crystal phases are in a separate section of the table. In most cases, these densities have not been fit as a function of temperature. Values of parameters, statistical measures of the fit, and references to sources of critical constants appear at the beginning of these sections.

Case 2. For data sets that do not meet the criteria of Case 1, but contain acceptable values over a temperature range of at least two degrees, the results are smoothed using a linear function of temperature with an estimated coefficient of thermal expansion. A table of smoothed recommended values is presented.

Case 3. For data sets that do not meet the criteria of either Case 1 or 2 but contain two or more values at a single temperature, a recommended value is given for this temperature by taking a weighted average of the observed values.

Case 4. For data sets that contain only single values at one or two temperatures, the reported values are given rather than recommended values.

1.4 Evaluation, Selection and Smoothing of Data

1.4.1 Assignment of Uncertainties

The Thermodynamics Research Center staff have assigned an uncertainty value to each observed and recommended density value listed in the tables. The true value of the property has a 95% probability of being in the range covered by + or – the uncertainty about the reported value. Assignment of uncertainty is a subjective evaluation based upon what is known about the measurement when the value is entered into the database, and includes the effects of all sources of experimental error. The errors have been propagated to the listed density at the reported temperature. Uncertainties reported by the investigators are considered but not necessarily adopted. Often, investigators report repeatability, but they usually do not provide uncertainty.

Errors in density result from errors in temperature measurement or control; calibration of instruments; transfer, handling and weighing of samples; and impurities in the samples. At temperatures well below the critical temperature and near room temperature, standard techniques easily achieve accuracies of $\pm 0.05\%$. For the compounds in this compilation, that level corresponds to about $\pm 0.4 \text{ kg}\cdot\text{m}^{-3}$. Under these conditions, errors in temperature are not very significant. This level of accuracy only requires

temperatures to be known within ± 0.5 K. At temperatures approaching the critical temperature, measurements become more demanding because of the rapid increase in the magnitude of the coefficient of thermal expansion. Greater accuracy, in general, requires careful attention to calibration, mass determination and sample handling techniques. It is assumed that values obtained by pycnometers have been corrected for buoyancy of air, unless the author specifically says otherwise. This correction increases the apparent density by 0.05 - 0.1%. When this correction has not been made, the estimated uncertainty is greater.

Most measurements of densities of liquids below their normal boiling points are made in the presence of air. Densities reported here refer to liquids in equilibrium with a gas phase consisting of a mixture or air and vapor at a total pressure of one atmosphere below the normal boiling point and of vapor at the equilibrium vapor pressure above the boiling point. Thus air is not regarded as an impurity.

A major source of error in most measurements is the presence of impurities in the sample. The effect of an impurity depends upon its amount in the sample and upon the difference between its density and the density of the principal constituent. Even when the sample purity is provided quantitatively, the impurities often are not identified individually. Nevertheless, a report of sample purity reduces the estimated uncertainty because it can be taken as evidence that the investigator has considered sample purity. The most ubiquitous impurity in liquids is water, and, because its density differs significantly from those of hydrocarbons, it is a common source of error. Exclusion of water requires that the sample be protected from the atmosphere during transfer, and that special precautions be taken to remove the sample from containers.

1.4.2 Quantitative Effect of Impurity on Density of Liquids

The molar volume of a mixture of components, V , in terms of the mole fractions x_i and partial molar volumes of the components V_i is:

$$V = \sum_{i=1}^c x_i V_i \quad (1.5)$$

For an ideal solution, the partial molal volumes equal the molar volumes of the pure liquid components. Denoting component the main components as 1 and the impurities as > 1 , the volume becomes:

$$V = x_1 V_1 + \sum_{i=2}^c x_i V_i. \quad (1.6)$$

Then using,

$$\rho = M / V \quad (1.7)$$

and the molar mass of the mixture:

$$M = \sum_{i=1}^c x_i M_i \quad (1.8)$$

and assuming that the x_i are small for $i > 1$, then

$$\rho = \frac{\rho_1}{w_1} \left(1 - \rho_1 \sum_{i=2}^c w_i v_i \right) \quad (1.9)$$

where $v_i = V_i/M_i$ are partial specific volumes of the impurities and w_i is the mass fraction of component i . Finally, the density of the mixture is related to the density of the main component and the impurities i by:

$$\rho = \frac{\rho_1}{w_1} \left(1 - \rho_1 \sum_{i=2}^c \frac{w_i}{\rho_i} \right) \quad (1.10)$$

The observed value of the density of a sample is sometimes presented as evidence of its purity. Assuming the sample contains a single impurity, equation (1.10) can be solved for $\rho - \rho_1$:

$$\rho - \rho_1 = \rho_1(1 - w_1 - \rho_1 w_2 / \rho_2) / w_1 \quad (1.11)$$

1.4.3 Procedure for Selection and Smoothing of Density Values - Case 1

A selected subset of the reported densities is fit to functions of temperature using the least squares criterion. Up to a boundary temperature T_b (approximately $0.8T_c$), the calculated density ρ_x is represented by a polynomial in temperature with coefficients a_k of order p ,

$$\rho_x = \sum_{k=0}^p a_k T^k. \quad (1.12)$$

Above T_b the smoothed values are given by a modification of the Guggenheim equation [67-gug]

$$\rho_x = \left(1 + 1.75\theta + 0.75\theta^3\right) \left[\rho_c + b_1(T_c - T) + b_2(T_c - T)^2 + b_3(T_c - T)^3 + b_4(T_c - T)^4 \right], \quad (1.13)$$

where T_c is the critical temperature and $\theta = (1 - T/T_c)^{1/3}$. Selected values of critical constants are constant. Continuity with equation (1.12) results from forcing the two functions and their first derivatives with respect to temperature to be equal at the boundary. When no values are available above this temperature, only the polynomial is used.

The following steps, implemented by a computer program written in C, generate the smoothed, recommended values. Input to the program consists of the set of observed density values, temperatures, estimated uncertainties, critical constants and values of certain parameters used by the program.

Step 1. Separate the initial data into two sets, corresponding to temperatures above and below T_b .

Step 2. Make an initial selection from the low temperature set by rejecting all points with zero uncertainty and all points with uncertainties above a limit determined by the data selection algorithm described in section 1.5.2. Zero uncertainties are assigned to values that are not experimental and are included for comparison only (these are most often values recommended in other compilations).

Step 3. Determine the effective number of data values, n_e , as described in 1.5.3. If the effective number of values is less than four, terminate the calculation. If the total number of values is more than eight and the effective number is greater than or equal to four but less than eight, make another initial data selection with relaxed selection criteria.

Step 4. For the j -th value in the set calculate normalized values, ρ_{nj} and $T_{n,j}$, and weighting factors, $w_j = 1/u_j^2$ where u_j is the uncertainty assigned to the j -th observed density and $\rho_{n,j} = \rho_j - \bar{\rho}$ where $\bar{\rho}$ is the mean value of the observed density in the set. and $T_{n,j} = T_j - \bar{T}$ where \bar{T} is the mean value of the T_j value in the set..

Step 5. Using $\rho_n = a_1 T_n$, fit the data subject to least squares with points weighted by w_j .

Step 6. Calculate the standard deviation σ for this fit. Eliminate any points from this set for which $|\delta_j| > 3.5\sigma$, where $\delta_j = \rho_j - \rho_{x,j}$.

Step 7. Fit the remaining normalized values to a series of polynomials, $\rho_n = \sum a_k T^k$, starting with order 1 and increasing in order. Use w_j as weighting factors and stop increasing the order when satisfying one of the following conditions:

1. A value of p given as an input parameter to the program is reached, or
2. $\chi_k^2 < 1.1[1 + 1/(n - k)]^2 \chi_{k-1}^2$ (see glossary of symbols) and the deviations pass the random deviation test (see 1.5.4).

Step 8. If any points have $|\delta_j| > 2.2\sigma$ for the final polynomial, eliminate these points and repeat step 7.

Step 9. Calculate parameter a_0 .

Step 10. Apply the initial data selection described in step 2 to the high temperature data set.

Step 11. Fit the selected high temperature data with the modified Guggenheim equation using least squares with weighting factors w_j .

Step 12. The following procedure provides continuity at the boundary. Set equation (1.13) and its first derivative at T_b equal to the corresponding values from equation (1.12) at T_b . Eliminate parameters b_3 and b_4 from these two simultaneous equations to obtain a function containing parameters b_1 and b_2 which can be evaluated for the high temperature range using least squares. Do not use densities at temperatures within 2 K of the critical temperature.

Step 13. Generate the output table of temperature, observed densities, estimated uncertainties, and difference between observed and calculated densities and arrange it in order of year of publication with authors. For data from a particular source, arrange in order of temperature.

Step 14. Calculate the table of smoothed and recommended values with their corresponding estimated uncertainties.

Coefficients A , B , C , D and E listed in the heading of Table 1 for each compound correspond to a_0 , a_1 , a_2 , a_3 and a_4 in equation (1.12) for temperatures below T_b . σ_i is the weighted standard deviation for individual points in this region (see the glossary). If the data set includes values above T_b , the coefficients A , B , C and D correspond to b_1 , b_2 , b_3 and b_4 in equation (1.13) for this range. The weighted standard deviation, $\sigma_{c,w}$, and the unweighted standard deviation for the fit, $\sigma_{c,uw}$, include both ranges. If the data set covers only values below T_b then $\sigma_{c,w}$ and $\sigma_{c,uw}$ represent that range only.

The uncertainty in the smoothed values depends upon the uncertainties in the original observed values and upon the magnitude of deviations between observed and calculated values. To approximate the contribution of these two effects at the temperature T , the uncertainties $u_x(T)$ for the low temperature range are calculated from:

$$u_x(T) = \left[u(T)^2 + \sum_k \sum_l C_{kl} (T^k - \overline{T^k})(T^l - \overline{T^l}) \right]^{1/2} \quad (1.14)$$

In this equation, $u(T)$ represents the uncertainty of the observed data in the vicinity of T and is approximated by fitting a polynomial of order 1-3 to the estimated uncertainties as a function of temperature (other symbols appear in the glossary). Uncertainties in the smoothed data for the high temperature range are calculated using:

$$u_x(T) = \left[u_x(T_b)^2 + h(T)^{-2} \right]^{1/2} \quad (1.15)$$

where $u_x(T_b)$ is the uncertainty calculated using equation (1.14) for the low temperature range at the boundary temperature T_b and $h(T)$ is a polynomial in temperature fit to the reciprocals of the estimated uncertainties in the high temperature region.

The uncertainties in extrapolated data should increase as the extent of extrapolation increases. Since equation (1.15) does not always give this result, manual adjustment is sometimes required in this range.

1.4.4 Procedure for Selection and Smoothing of Density Values - Case 2

When the data set for a particular compound satisfies the criteria for Case 2, it is smoothed by a linear function of temperature,

$$\rho_x = a_0 + a_1 T \quad (1.16)$$

The coefficient a_1 is either calculated from two densities of sufficient accuracy reported at different temperatures, preferably by the same investigator, or estimated by examination of the coefficient of expansion of similar compounds obtained from a least squares calculation. The constant term then results from equation (1.17) after eliminating values with large uncertainties

$$a_0 = \sum w_j (\rho_j - a_1 T_j) / \sum w_j \quad (1.17)$$

The uncertainties for the smoothed values are:

$$u_x(T) = [\sigma_0^2 + \sigma_1^2 (T - \bar{T})^2]^2 \quad (1.18)$$

where \bar{T} is the weighted mean temperature for the accepted set, $\sigma_0^2 = (\sum w_j \delta_j^2) / \sum w_j$ and σ_1 is the estimated standard deviation of a_1 .

1.4.5 Procedure for Selection and Smoothing of Density Values - Case 3

The recommended density at a particular temperature is the weighted mean observed density for that temperature. The corresponding uncertainty is the standard deviation from the mean for each value.

1.5 Calculation Procedures

1.5.1 Least Squares Calculation

Parameters of all the smoothing functions are adjusted to minimize the function

$$\chi^2 = \sum w_j \delta_j^2 \quad (1.19)$$

by the singular value decomposition of the matrix of independent variables of the function. The parameters are calculated by functions **svdcmp** and **svbksb** described in [88-pre/fla] modified to accept weighting factors. The covariance matrix used in equation (1.14) is calculated by the function **covar** from the same book.

1.5.2 Selection of Data Based upon Estimated Uncertainties

The selection procedure is:

Step 1. Obtain ΔT , the range of temperatures covered by the data set.

Step 2. For each density value, ρ_j , in the set, calculate,

$$x_{jl} = \exp\left(q|T_j - T_l|\right) \quad (1.20)$$

$$z_1 = \sum_{l \neq j} x_{jl} \quad (1.21)$$

$$z_2 = \sum_{l \neq j} u_l x_{jl} \quad (1.22)$$

$$y = u_j z_1^{1.5} z_2^{-1} \quad (1.23)$$

Accept point j if $y \leq d$; reject it otherwise

Step 3. Repeat steps 1 and 2 with points accepted in the first pass.

The accepted points are those that remain from Step 3. The constants q and d are:

$$q = -2.628 g_1 \left[1 + (\Delta T / 30)^2 \right] / \Delta T$$

$$d = g_2 / \log_{10}(1 + n)$$

The number z_2 / z_1 is a weighted mean of all points in the set other than the j -th point. The weighting factor decreases exponentially with the difference in temperature of the l -th point from the j -th point. The parameter g_1 determines the rate of decrease. This procedure compares the uncertainty of the j -th point to the weighted mean of other points. The parameter g_2 determines the rejection level from this comparison for the j -th point. Larger values of g_2 are less selective. Values for g_1 and g_2 are supplied to the algorithm. For all cases g_1 is in the range of 1 to 2 (usually 1.8). The value of g_2 is in the range of 2 to 3 (kg·m⁻³) (usually 2.5).

1.5.3 Count the Effective Number of Density Values in a Set

The number of degrees of freedom in a least squares fit is the number of distinct data values minus the number of adjustable parameters. To obtain a meaningful smoothing of data, the order of the polynomial function is limited to values which gives three or more degrees of freedom. However, if two or more density values in the set are at the same (or nearly the same) temperature, they should count as only one point in calculating the degrees of freedom. In general, the effective number of density values minus the number of fitting parameters is used as the degrees of freedom. Effective data values are those that are separated by at least 1.2 K.

1.5.4 Testing a Set of Deviations between Observed and Calculated Density Values for a Random Distribution

One of the criteria for acceptance of the order of a polynomial least squares fit is that the deviations between calculated and random values be distributed “randomly” over the range of conditions covered by the data. The concept of randomness for this purpose probably cannot be defined rigorously. However, the following test for randomness is used whenever the original data set contains seven or more values.

Step 1. Sort the values in order of increasing temperature

Step 2. Separate the total range of temperature, ΔT , into s subranges each of size $\Delta T/s$. Form s subsets of data corresponding to these temperature subranges.

Step 3. Make the following comparison for each subset j which has at least four members.

$$0.01 < \frac{\sum |\delta_j|}{n_s} \quad \text{and} \quad 0.2 < \frac{|\sum \delta_j|}{\sum |\delta_j|}$$

If both comparisons are true for any subset, the test for randomness fails.

Step 4. Apply steps 2 and 3 to the data for s from 2 to an upper limit. The upper limit is determined by the number of values in the original set according to the following table.

n , number of values in original set	maximum number of subsets
7 to 10	2
11 to 20	3
21 to 33	4
> 33	5

1.6 Glossary of Symbols

a_k	parameters in the polynomial function for densities at temperatures $\leq T_b$
b_k	k -th parameter in modified Guggenheim equation for density at temperatures $> T_b$
g_1, g_2	parameters used in the data selection algorithm
n	number of accepted values of density in a set
n_e	effective number of accepted values of density in a set
n_s	number of density values in subset s
p	order of the polynomial for density values at temperatures $\leq T_b$
s	number of subsets in the random deviation algorithm
u_j	uncertainty assigned to the j -th observed density value in a set
w_j	weighting factor for the j -th density value in a set
$C_{k,l}$	Element k,l of the variance-covariance matrix for the polynomial parameters
T	absolute temperature
T_b	boundary temperature
T_c	critical temperature
T_j	temperature for the j -th observed density
$\overline{T^k}$	mean value of the T_j^k values in a set
$T_{n,j}$	$T_j^k - \overline{T^k}$, normalized value of the j -th temperature raised to the k power
δ_j	$\rho_j - \rho_{x,j}$
θ_j	$(1 - T_j/T_c)^{1/3}$
ρ	density
$\rho(\text{API})$	API specific gravity
$\bar{\rho}$	mean value of observed densities in a set
ρ_0	density of a standard substance
ρ_c	critical density

ρ_j	observed value of j -th density in a data set
ρ_m	molar density
$\rho_{n,j}$	$\rho_j - \bar{\rho}$, normalized density for the j -th value
ρ_r	relative density
$\rho_{x,j}$	calculated value of the j -th density in a data set
σ	$(\chi^2/n)^{1/2}$, standard deviation for density values in a set
χ_k^2	$\Sigma \delta_j^2$ for all values in a set fit to a polynomial of order k
ΔT	$T_n - T_1$, range of temperatures for data in a set

The following symbols refer to components in a mixture at a fixed temperature:

c	number of components in the mixture
i	component number
v_i	partial specific volume of component i in the mixture
w_i	mass fraction of component i in the mixture
x_i	mole fraction of component i in the mixture
M_i	molar mass (molecular weight) of component i
V	molar volume of a mixture
V_i	partial molal volume of component i in the mixture
ρ	density of a mixture of components
ρ_i	density of pure component i

Symbols used in the tables:

A, B, C, D, E	coefficients in function for density (see section 1.4.3)
ρ_{calc}	calculated density, ρ_x
ρ_{exp}	observed value of j -th density in a data set, ρ_j
σ_t	$(\Sigma w_j \delta_j^2 / \Sigma w_j)^{1/2}$, for low temperature range only
$\sigma_{c,w}$	$(\Sigma w_j \delta_j^2 / \Sigma w_j)^{1/2}$, for low and high temperature range combined
$\sigma_{c,uw}$	$[\Sigma \delta_j^2 / n(n-p-2)]^{1/2}$, for low and high temperature range combined
$2\sigma_{\text{est}}$	estimated uncertainty, u_j

1.7 Compound Nomenclature

1.7.1 Order of Compounds in the Tables

The density tables are organized into 5 main classes of compounds as described in the Table of Contents. The first 4 classes represent increasing closeness of bonding between the hydrocarbon rings. The 5-th class contains miscellaneous compounds of mixed types. Within each main class there are two or more subclasses. They start with fully saturated compounds and proceed with increasing extents of unsaturation. Within each subclass the compounds are arranged in formula order. First with increasing number of carbon atoms in the empirical formula and then with increasing number of hydrogen atoms. Compounds with the same formula are sorted alphabetically by Table Name.

1.7.2 Names of Compounds Used in the Tables

Polycyclic hydrocarbons may be named in a variety of ways. These include several kinds of systematic names, recommended by the International Union of Pure and Applied Chemistry (IUPAC) [93-ano-1], indexing names used by *Chemical Abstracts*, and various trivial and other names found in the chemical literature.

Stereoisomers are identified by various prefixes. (*E*)- and (*Z*)- indicates the relative orientation of groups attached to two carbons connected by a double bond, according to IUPAC rules. *Cis*- and *trans*- indicate the relative orientation of groups attached to non-aromatic rings. In cases of multiple substitution the orientation is indicated by (*R*)- and (*S*)-. Saturated fused ring systems exist in *cis*- and *trans*- forms which correspond to the relative orientation of the hydrogen atoms attached to the two bridgehead carbon atoms. Stereo information is included when given in the original documents. More often however particular stereoisomers are not identified. In most such cases the samples are mixtures of stereoisomers. Generally the difference between the density of liquid stereoisomers is less than 1%. The difference is less for high molecular weight compounds..

A standard style is used to assign names of compounds in the tables of density data. These are called Table Names. These names, along with other kinds of names are included in the Chemical Name Index provided at the end of the volume.

Systematic names describe the molecular structure of a compound. A systematic name consists of two parts, <substituents><parent>. The <parent> is the name of a compound having a particular carbon skeleton. The <substituents> are a list of one or more radical groups connected by chemical bonds to the parent compound. Substituents are arranged in alphabetical order within a compound name. If the parent contains more than one carbon atom, each substituent name is preceded by a number identifying the carbon atom in the parent compound to which it is connected.

A *Chemical Abstracts* indexing name is formed by inverting a systematic name, in the form <parent>, <substituents>-. Whenever a Chemical Abstracts Registry Number can be found for a compound it is listed along with the formula and Table Name. *Chemical Abstracts* gives an indexing name for each of these compounds, and sometimes other names that have been used in the literature. When a registry number assigned by *Chemical Abstracts* cannot be found a number, starting at 50000-00-0, used for identification in the TRC SOURCE database is given.

Trivial names do not carry any structural information.

A Table Name is a systematic name recommended by IUPAC. The style used to generate Table Names is described as follows.

Class 2.1 Saturated alicyclic rings attached to aliphatic chains.

These compounds are named as cycloalkylalkanes. Examples are dicyclohexylmethane, 1,5-dicyclopentylpentane, 1-cyclohexyl-3-(2-methylcyclohexyl)propane.

Class 2.2 Unsaturated alicyclic rings attached to aliphatic chains

These consist of three types: cycloalkenylalkanes, cycloalkadienes, cycloalkynes, *etc.* (unsaturation in the ring), cycloalkylalkenes, (unsaturation in the side chain) and cycloalkenylcycloalkenes (unsaturation in both ring and side chain). Example: 2-cyclohexyl-2-(cyclohexen-3-yl)propane.

Class 2.3 Alicyclic and phenyl rings attached to aliphatic chains

These include both saturated and unsaturated rings and chains. Examples: 1-cyclopentyl-2-phenylethane, 1-(1-cyclohexenyl)-2-phenylethane, 1-cyclohexyl-2-phenylethane

Class 2.4 Phenyl groups attached to saturated aliphatic chains

The parent is an alkane and the substituents are phenyl and alkyl radicals.
Examples: 1,2-diphenylbutane, 1,1-diphenyl-2-methylpropane

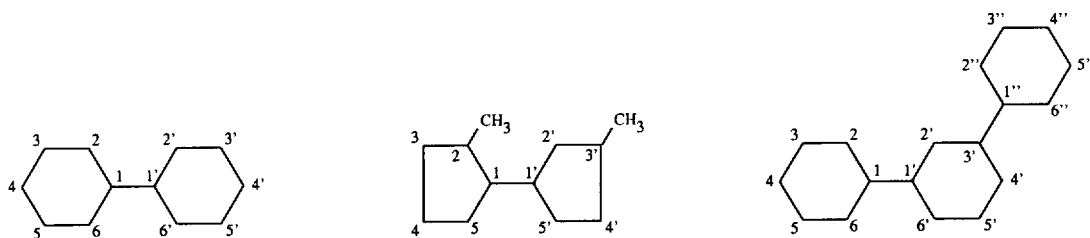
Class 2.5 *Phenyl groups attached to unsaturated aliphatic chains*

The parent is an alkene or alkyne and the substituents are phenyl and alkyl radicals.

Examples: 1,3-diphenyl-1-propene, *cis*-2,3-diphenyl-2-butene, 2,3-diphenyl-1,3-butadiene.

Class 3.1 *Saturated polycycloalkyls*

Class 3 consists of compounds in which two rings are joined by one chemical bond between carbon atoms from each ring. Names of saturated compounds are alkyl-1,1'-bicycloalkyls, and alkyltercycloalkyls. Position numbers of the different rings are distinguished by use of primes. Thus,



1,1'-bicyclohexyl

2,3'-dimethyl-1,1'-dicyclopentyl

1,1':3,1''-tercyclohexyl

Class 3.2 *Unsaturated polycycloalkyls*

Named as cycloalkylcycloalkenes, or cycloalkenylcycloalkanes. Example: 2-cyclohexylcyclopentene.

Class 3.3 *Alicyclic rings attached to phenyl groups.*

These are named as phenylcycloalkanes, phenylcycloalkenes, or cycloalkylbenzenes. The style depends on the number of cycloalkyl and phenyl groups.

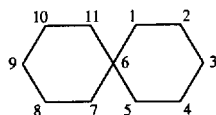
Class 3.4 *Compounds of two or more phenyl rings.*

Parent compounds are 1,1'-biphenyl, and various terphenyls. Position numbers on the different rings are distinguished by use of primes, as for polycycloalkyls.

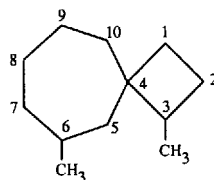
Examples: 2-ethyl-1,1'-biphenyl, 3,4'-dimethyl-1,1'-biphenyl.

Class 4.1 *Spiroalkanes and Spiroalkenes*

In this class two rings are joined by a carbon atom common to both. The Table Name follows Method 1, Rule A-41 of the IUPAC recommendations [93-ano-1] The parent compound for saturated hydrocarbons is named *spiro*[*n.m*]alkane. Substituents are alkyl radicals. The alkane part indicates the total number of carbon atoms in the two rings combined. Numbers, *n* and *m* are the number of carbon atoms in the two individual rings, not counting the common atom. Carbon atoms in the rings are numbered starting with the one next to the common atom in the smaller ring and continuing on through the smaller ring and then through the larger ring.



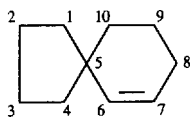
Spiro[5.5]undecane



3,6-dimethylspiro[6.3]decane

Class 4.2 Unsaturated Spiroalkanes

Example: Spiro[4.5]-6-decene

**Class 5 Condensed Ring Systems**

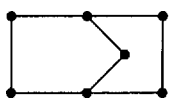
Condensed Ring Systems contain two or more pairs of rings joined by two carbon atoms in common. These are the bridgehead atoms. IUPAC [93-ano-1] recommends two general methods of naming these compounds. In Method 1, described by Rule A-21 the parent compound is given a trivial name for a polycyclic aromatic hydrocarbon. Partially or completely hydrogenated compounds are named by the use of “hydro” as a substituent. The name perhydro indicates complete hydrogenation. Other substituents may be alkyl-, cycloalkyl-, and benzo- radicals.

Position numbers on the rings are assigned by first orienting the system in a manner described by the rule. The carbon atom next to the bridgehead atom in the upper right hand ring is assigned the number ‘1’. Increasing numbers are assigned to atoms in a clockwise manner around the ring system back to the starting atom. Bridgehead atoms are numbered as *na*, *nb*, .. where *n* is the number of the preceding atom in the ring.

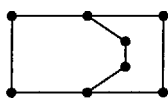
In Method 2, described by Rule A-31, the saturated cyclic parent is named as a polycyclo-[..]alkane. The alkane name identifies the total number of carbon atoms in the ring system. The names bicyclo, tricyclo, tetracyclo, *etc.* identify parent compounds of two, three, four, *etc.* rings. Double bonds in the ring are identified by names such as *n*-alkene, *n,m*-alkadiene, where the *n* and *m* give the position of the double bond. Substituents consist of alkyl, cycloalkyl, phenyl, *etc.* radicals.

Compounds with two rings have three paths between the two bridgehead atoms. The numbers in brackets identify the number of carbon atoms between the two bridgeheads. Each additional ring is characterized by an additional path joining two atoms, which serve as additional bridgehead. These additional paths are identified by the number of carbon atoms between the two atoms, with a superscript that identifies the position numbers of the two bridgehead atoms.

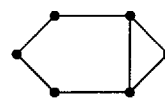
In Method 2, position numbers in the rings are obtained by assigning number ‘1’ to one of the bridgeheads and continuing in sequence around the largest path back to the second bridgehead atom, then around the largest remaining path back to the beginning position and finally through the shortest path. Some examples:



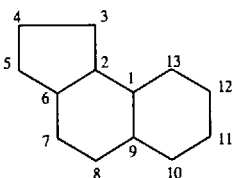
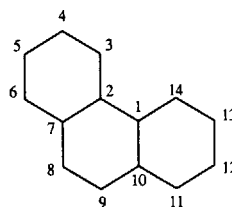
Bicyclo[2.2.1]heptane



Bicyclo[2.2.2]octane

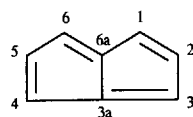


Bicyclo[3.2.1]octane

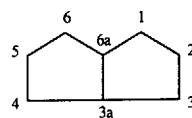
Tricyclo[7.4.0.0^{2,6}]tridecaneTricyclo[8.4.0.0^{2,7}]tetradecane

Shown below are the aromatic ring systems and names of compounds in this book used for Method 1. There are two types of these. The *ortho*-fused and the *ortho*- and *peri*-fused rings. For each of the *ortho*-fused ring systems the corresponding saturated ring system and the name obtained by Method 2 is shown.

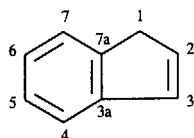
Ortho-fused compounds:



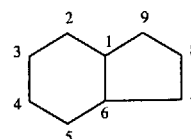
Pentalene



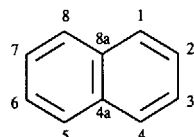
Bicyclo[3.3.0]octane



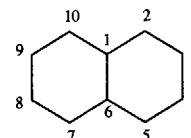
1H-Indene



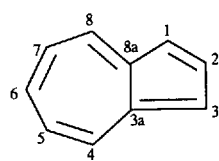
Bicyclo[4.3.0]nonane



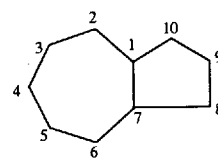
Naphthalene



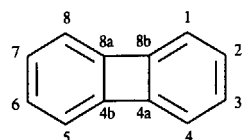
Bicyclo[4.4.0]decane



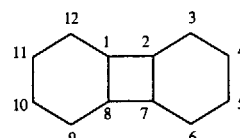
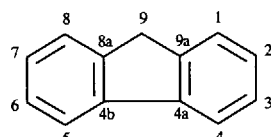
Azulene



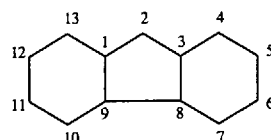
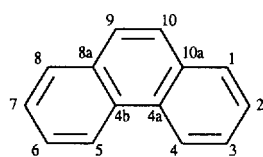
Bicyclo[5.3.0]decane



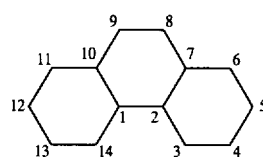
Biphenylene

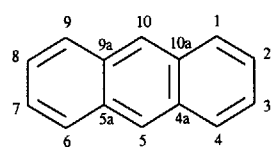
Tricyclo[6.4.0.0^{2,7}]dodecane

9H-Fluorene

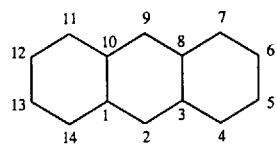
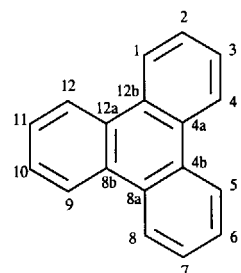
Tricyclo[7.4.0.0^{3,8}]tridecane

Phenanthrene

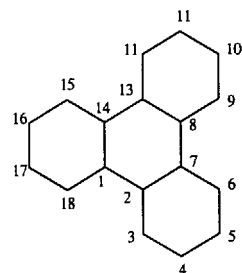
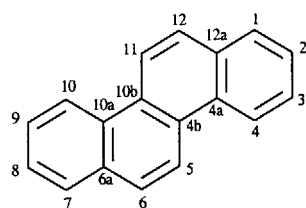
Tricyclo[8.4.0.0^{2,7}]tetradecane



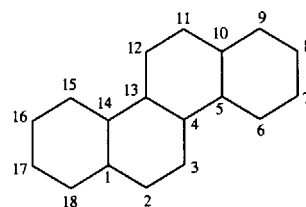
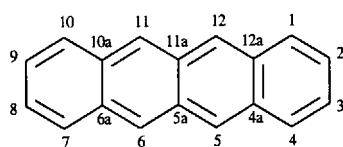
Anthracene

Tricyclo[8.4.0.0^{3,8}]tetradecane

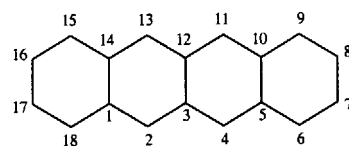
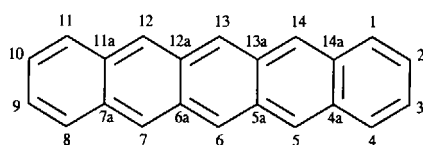
Triphenylene

Tetracyclo[12.4.0.0^{2,7}.0^{8,13}]octadecane

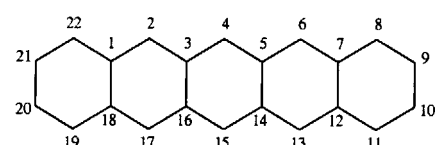
Chrysene

Tetracyclo[12.4.0.0^{4,13}.0^{5,10}]octadecane

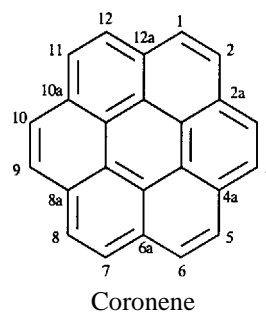
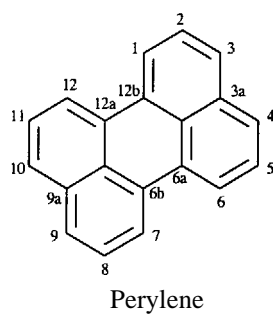
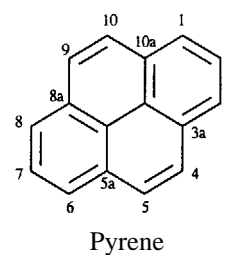
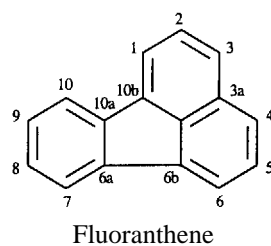
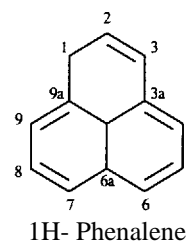
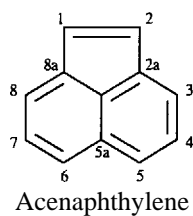
Naphthacene

Tetracyclo[12.4.0.0^{3,12}.0^{5,10}]octadecane

Pentacene

Pentacyclo[16.4.0.0^{3,16}.0^{5,14}.0^{7,12}]docosane

Ortho- and *peri*-fused compounds:



Method 1 is used for the Table Names of compounds and their derivatives in the list above. Method 2 is used for other fused-ring compounds. Several examples of Method 1 and Method 2 names for the same compounds are:

Method 1	Method 2
2,3-Dihydro-1H-indene (also called indan)	Bicyclo[4.3.0]-2,4,(5,9)-nonatriene
Octahydro-1H-indene (hexahydroindan)	Bicyclo[4.3.0]nonane
1-Methyl-1,2,3,4-tetrahydronaphthalene	7-Methylbicyclo[4.4.0]-2,4,(6,10)-decatriene
Decahydro-2-methylnaphthalene	3-Methylbicyclo[4.4.0]decane
Decahydro-1-ethyl-5-methylnaphthalene	2-Ethyl-7-methylbicycl[4.4.0]decane
1-Methylperhydrophenanthrene	6-Methyltricyclo[8.4.0.0 ^{2,7}]tetradecane

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