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CHREV. 167

APPLICATIONS OF TWO-DIMENSIONAL THIN-LAYER CHROMATOGRAPHY

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(First received January 5th, 1983; revised manuscript received January 25th, 1983)

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1. INTRODUCTION

Bi-directional chromatography, which is a more specific term than two-dimensional chromatography when referring to flat paper or thin-layer beds[1], is an analytical technique that is becoming increasingly important in the separation of mixtures of varying complexity. This method consists in spotting a sample at the corner of a flat bed and allowing the migration of a solvent in one direction, followed by another migration at right-angles to the first.

When the same solvent is fed successively in the two directions of a uniform adsorbent layer, all chromatographed spots align on a diagonal. The sole advantage of the method is then a very slight increase in resolution corresponding to an increase, by a factor of $\sqrt{2}$, in the distance of migration of the spot. The realization of more efficient systems, by means of which a larger number of spots can be resolved[2], implies the use of the entire chromatographic area available and requires the selection of appropriate different mobile phases for each direction.

Similar efficiencies are attained when the same mobile phase is fed successively, at an orthogonal angle, to a chromatographic plate that has been coated with two adsorbents. Different retention mechanisms dictate the behaviour of the solutes chromatographed for instance, on a reversed-phase layer in one direction and a normal-phase layer in the other. The solute R_F values are then different in each direction and the spots are dispersed on the chromatographic plate.

The tremendous separation potential afforded by this technique is apparent from the flexibility available in combining various stationary and mobile phases for use in either direction.

In 1944, Consden, Gordon and Martin[3] first reported a bi-dimensional separation of amino acids on paper. The eluents used were collidine–water in one direction and phenol–water in the second. The chromatography took 5 days and resulted in the resolution of 15 of the 22 amino acids in the sample mixture. This technique was subsequently described by Overell[4], Cheftel *et al.*[5] and Nordmann *et al.*[6,7], who successfully achieved the separation of various organic acids.

The importance of this method increased in the early 1950s as bi-directional chromatography became instrumental in the elucidation of several biochemical pathways[8]. Calvin[9,10], for instance, used two-dimensional paper chromatography in combination with autoradiography to assay algal extracts kept in air containing $^{14}CO_2$. After the identification of the various sample components, a kinetic study of ^{14}C incorporation helped to suggest a scheme for carbon reduction during photosynthesis. The same technique enabled Beloff-Chain *et al.*[11,12] to differentiate between the conversion of glucose into oligosaccharides, polysaccharides and lactate in muscles and that into amino acids and lactate in the brain. Chain *et al.*[13,14] also studied the effect of insulin on glucose metabolism in various types of animal tissue such as the diaphragm, liver, brown adipose tissue, brain and the pituitary.

Although two-dimensional thin-layer chromatography (2-D TLC) has been used for almost 40 years (Fig. 1), there has been no review of its various applications prior to this paper. Several workers have reported past and present developments of classical TLC and its future trends[15–20]. The performance and spot capacity of two-dimensional TLC have been described elsewhere[21], and also recent developments in TLC instrumentation[22].

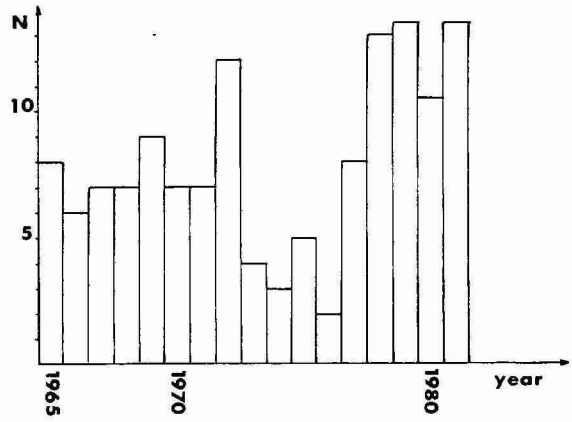


Fig. 1. Histogram showing the number of original two-dimensional TLC publications in the last 18 years.

This paper briefly reviews the different types of stationary phases available for chromatography, and the effective mechanisms of solute retention on each phase, prior to discussing the various applications of the 2-D technique. A short discussion on the methods available for spot detection is also included.

We have tried to cover the literature as thoroughly as possible. Authors who have not been cited are kindly asked not to take offence but rather to inform us of their work. More importantly, this review aims to demonstrate the efficiency of the method in resolving compounds of widely different nature, polarity or class, and the importance of the judicious selection of chromatographic conditions such that different mechanisms may govern solute retention in each direction.

2. STATIONARY PHASES AND RETENTION MECHANISMS

Various powders are commercially available that may be slurried alone or admixed with agents for specific applications, and spread on glass, aluminium foil or plastic supports. Pre-coated TLC plates are also available without or with a binder for increased adhesion and mechanical stability of the layer, or an indicator for solute detection.

The thickness of the layer is often 0.1–0.3 mm for analytical applications and 0.5–2.0 mm for preparative work. The particle size varies, a small diameter being less critical than a narrow size distribution in achieving high efficiencies and good resolution[2]: the narrow size range, 5 μm "HPTLC" packings have disadvantages such as a slow flow-rate of the mobile phase, a long development time and spot diffusion, whereas packings with the same size distribution and a larger diameter (10–20 μm) afford faster and still adequate separations[2,23], as is obvious from results obtained with good but conventional TLC plates made with particles *ca.* 11 μm in diameter[24].

The type of stationary phase needed to resolve a given mixture depends, to a large extent, on the properties of the sample components. In general, stationary phases may be inorganic sorbents (silica, alumina, magnesia), organic sorbents (cellulose, polyamide), ion exchangers (ionic moieties substituted on to an organic adsorbent) and reversed phases (non-polar, organic groups chemically bonded often to an in-

organic silica backbone). These thin layers may be impregnated with a specific reagent to enhance or create a particular type of solute–stationary phase interaction, or coated side-by-side on a support, a practice often used in bi-directional TLC.

2.1. Inorganic adsorbents

Inorganic oxides such as silica, alumina and magnesia are polar adsorbents which, according to their degree of activation, may be used to separate polar or moderately polar compounds. Procedures for adsorbent activation by heat or deactivation by addition of a moderator such as water have been standardized to ensure reproducibility of separations.

Heat activation rids TLC plates of physically adsorbed water, thus freeing the adsorptive surface for interactions with various solutes. Adsorptive sites in silica and magnesia are essentially hydroxyl groups. Thus, heating these two adsorbents to temperatures above 200°C for silica and 100°C for magnesia, a process whereby Si–OH and Mg–OH groups are converted into Si–O–Si and Mg–O–Mg, respectively, results in the loss of chromatographic activity[25]. In alumina, active adsorptive sites are thought to be aluminium atoms, strained Al–O bonds, basic oxide ions and cationic centres. The loss of most of the surface hydroxyl groups early in the heating process does not reduce the activity of alumina, which actually increases with increasing temperature up to about 800°C and is lost only at 1000°C[25].

In chromatographic systems that involve weak or moderately strong solvents, adsorption is described primarily by the following relationship[25]:

$$\log K = \log V_a + \alpha (S^0 - A_s \varepsilon^0) \quad (1)$$

where K, the distribution coefficient, is the ratio of the solute concentration in the adsorbed state to that in the mobile phase, V_a is the volume of a monolayer of solvent adsorbed on the surface, α, the activity of the adsorbent, is proportional to its average surface energy and related to its water content, S^0 is the adsorption energy of the solute in the reference solvent and on an adsorbent of standard activity ($\alpha = 1$), A_s is the molecular area required for the adsorption of a solute molecule on the adsorbent surface and ε^0 is the solvent strength parameter[25].

Hence, the extent of retention by adsorption on a given phase increases primarily with the activity, average surface energy and surface area of the adsorbent. In addition, retention increases with S^0, the adsorption energy of the solute molecule, which is approximately equal to the sum of the individual adsorption energies contributed by each constituent group. Certain functional groups interact more strongly with polar adsorbents than others. The retention, for the corresponding solutes, increases in the order saturated hydrocarbons < aromatic hydrocarbons ≈ halogen derivatives < ethers < esters ≈ aldehydes ≈ ketones < amines ≈ alcohols < carboxylic acids.

Stronger solvents (larger ε^0) decrease the solute retention. This effect is more important for larger solute molecules (large A_s, eqn. 1). The polarity of the mobile phase needed to achieve adequate R_F values is determined by that of the solutes studied. Polar compounds often require the presence of water in the mobile phase to ensure the *in situ* deactivation of the plate and prevent the occurrence of tailing or

irreversible chemisorption caused by strong adsorbent–solute interactions. In addition, desorption is ensured by the favoured interactions of the solute with the polar eluent. However, when the amount of water in the eluent exceeds 16%, solute partition is effective to a certain extent[26].

Other factors that affect adsorptivity are the acidic or basic functionalities of the adsorbent, as well as steric factors. Each adsorbent is characterized by a definite geometrical arrangement of adsorptive sites, favouring interaction with certain types of solutes. For instance, alumina is better suited than silica for the separation of aromatic hydrocarbons with different functional groups or steric arrangement. Moreover, although the adsorptive properties of alumina are similar to those of magnesia, the latter adsorbent has a much higher affinity for carbon–carbon double bonds and is especially suitable for the separation of planar aromatic hydrocarbons.

In general, solute interactions with a given adsorbent may involve London dispersion forces, orientation or induction dipole forces, hydrogen bonding and weak covalent bonding (acid–base interactions and complex formation). The extent to which any of these occurs depends on the particular chromatographic system used. Adsorbents may often be impregnated with specific reagents that may complex reversibly with the solute or covalently bond to it. Impregnation with boric acid, for instance, is used for the separation of vicinal dihydroxy isomers which are retained by forming cyclic boric acid derivatives. Argentation chromatography or impregnation with silver nitrate allows the separation of unsaturated compounds owing to rapid and reversible complexation of their π double bond electrons with the impregnated silver ions. Similarly, the separation of nitrogenous bases on plates impregnated with Zn, Cd or Mg involves the occurrence of selective interactions between the metal ion used and the free nitrogen electrons[19].

2.2. Organic sorbents

In addition to the aforementioned inorganic sorbents, various organic macromolecular stationary phases are also commercially available. Of these, polyamide and cellulose are the most commonly used, and are particularly suitable for the separation of hydrophilic, strongly polar substances.

2.2.1. Polyamide

With aqueous or polar eluents, this sorbent behaves as a reversed phase, whereupon partition is thought to be involved, at least to some extent, in solute retention. With non-polar developers, polyamide is a normal phase on to which chromatographed substances may adsorb. This adsorption may entail the function of hydrogen bonds between proton-donating groups such as hydroxyl, amino, carboxylic or phosphoric in the solute molecule and carbonyl oxygens in the sorbent. Additional interactions may occur between electrophilic nitro compounds, quinones or aldehydes and amino groups in the polyamide phase. Compounds with delocalized π electron systems are also found to exhibit strong affinity for the sorbent. Clearly, chromatography on polyamide is a process of simultaneous e^- donor–e^- acceptor interactions, the extent of which depends on the chemical nature of the solute, the composition of the desorbing eluent and the presence of free –NH– and $>C=O$ groups on the adsorbent surface[26].

2.2.2. Cellulose

In paper chromatography, one often witnesses rapid spreading of substances along cellulose fibres. The powdered sorbent used in TLC, however, is characterized by very short fibres which afford sharper spots and a better resolution. TLC cellulose exists in two forms: native fibrous (fibre length 2–25 μm, average degree of polymerization 400–500) and microcrystalline (particle size 20–40 μm, average degree of polymerization 40–200). In cellulose, most glucose units constitute crystalline regions, joined together as fibrils. These are bound into fibres by amorphous β-glucoside linkages. Whereas the crystalline surface is impermeable to most solvents, the amorphous regions hold imbibed water. Both structural types are responsible for solute retention, the former involving adsorption and the latter partition.

As partition involves the distribution of a solute between two immiscible liquids, it may be surprising at first to evoke this mechanism when solvents miscible with water, if not water itself, are used as developers. However, the water present in the amorphous regions has different properties to bulk water: it is linked by hydrogen bonds to the cellulose, forming a "liquid gel" with high apparent density and low velocity of diffusion.

The partition coefficient, a measure of solute retention, is determined by the extent of solute incorporation in the gel and interaction, by means of hydrogen bonds, with the "liquid gel" water. Molecular size and shape and the position and nature of hydrophilic groups in the chromatographed substance are important in this process[26].

Partition is not, however, solely responsible for chromatographic behaviour, as the migration sequence of several solutes differs from that based on partition coefficients alone. Adsorption and, to some extent, ion exchange are thought to participate in the chromatographic process.

2.3. Reversed phases

TLC layers for reversed-phase applications were first obtained by impregnating polar plates with organic solvents such as paraffin[27]. Normal phases were later chemically modified, *e.g.*, by the *in situ* acetylation of cellulose or silanization of silica plates. The resulting phases could withstand development in a wide variety of solvents, and ensured reproducibility of separations[28–30]. The number of commercially available reversed-phase plates increased subsequent to the more recent development of non-polar powders, in which different aliphatic chains are chemically bonded to a silica backbone. Halpaap *et al.*[31] tested such phases with respect to their chemical and physico-chemical characteristics, wettability and chromatographic retention data.

The mechanisms of solute retention on these various packings are diverse: partition is responsible for chromatography on paraffin-coated silica layers; with acetylated cellulose, although adsorption cannot be excluded, solutes are thought to partition, when aqueous eluents are used, between the mobile phase and the water-impregnated cellulose fibres; adsorption due mainly to solvophobic forces is responsible for solute retention on silanized or alkyl-chain bonded silica phases. However, when water is used in large amounts, especially with small-chain reversed phases, mixed-mode mechanisms are believed to occur.

2.4. Ion exchangers

Polystyrene sulphonic (Dowex 50) or amine (Dowex 1) resins have long been used in TLC work. However, polyacrylamide gels or carbohydrate (cellulose and dextran) polymers, whether chemically modified or impregnated with liquid ion exchangers, are more suitable for the separation of bulky solutes, such as proteins and nucleic acids. Compared with resin exchangers, these matrices have larger pores which allow a greater capacity and a better transfer of macromolecules. In addition, the greater spacing between the active sites helps to achieve selective desorption under milder conditions than with resin phases.

The moderately strong polyethyleneimine (PEI) and weak diethylaminoethyl (DEAE) cellulose basic anion exchangers are commonly used in TLC applications, as well as the strong sulphoethyl (SE) and weak carboxymethyl (CM) Sephadex (polydextran) acidic cation exchangers. Inorganic cation exchangers such as zirconium(IV) phosphate and ammonium molybdate, are also commercially available.

The affinity of a compound for an ion exchanger is known to be proportional to its charge. Besides the electrostatic forces which contribute mainly to chromatographic retention in ion exchange, additional interactions are often operative as in the physical adsorption of hydrophobic solute moieties on the skeleton of the exchanger. With weakly acidic and weakly basic phases, the pH of the eluent may affect selectivity as the exchanging groups ion pair with H^+ or OH^- ions in the solution[32].

2.5. Thin-layer gel chromatography phases

Dextran gels such as Sephadex G-10, admixed with silica gel or cellulose, have been used as TLC layers for the separation of purine and pyrimidine nucleotides and bases, for instance. While the character of the separations remains that of Sephadex, the layer has mechanical properties similar to those of silica gel or cellulose. Polyacrylamide gels (Biogel P) have also been used in TLC[33].

2.6. Stationary phases for two-dimensional thin-layer chromatography

Different sorbents may be slurried together and spread homogeneously on a plate for two-dimensional TLC purposes. The composition of the eluents is chosen such that, in each direction, a different sorbent interacts primarily with the solutes. Sorbents have also been coated side-by-side, forming coupled, two-phase plates; chromatography is then performed on a different phase in each direction.

The development of a plate in a given solvent is well known to affect the solute R_F values obtained from a subsequent development in another direction (Fig. 2). In addition, if the second solvent is very different from the first, its ascent in the orthogonal direction may be irregular, leading to distorted spots. In order to correct for those problems, Randerath and Randerath[35], after developing a PEI-cellulose plate in a buffer solution, washed away the residual salts by immersing the plate in methanol prior to a second elution. Bond[36] chose to transfer the spots obtained from the first development of a cellulose sheet on to another plate by clamping both thin layers face to face and developing with the second solvent, in a direction perpendicular to the first elution. The resulting chromatogram showed no interferences. In addition, the solute R_F values were unaffected by the previous run.

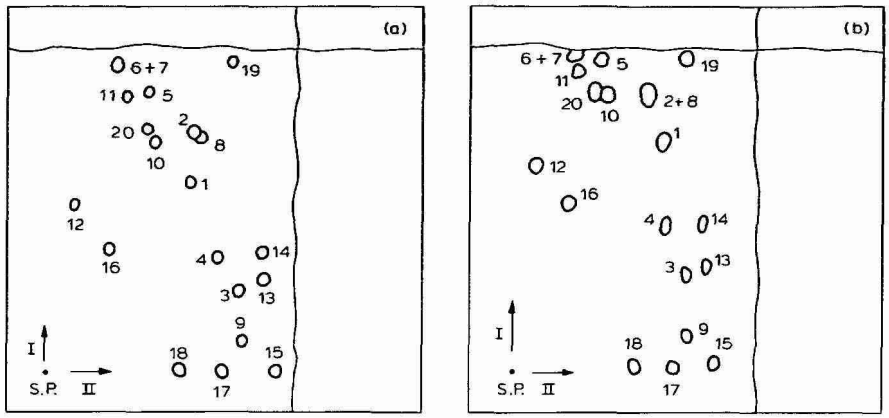


Fig. 2. (a) Theoretical and (b) experimental two-dimensional chromatograms of dinitrophenyl (DNP) amino acids on RP-18 plates. *Eluents: in the first direction, hexane–ethyl acetate–acetic acid (80:18:2); in the second direction, 1 M ammonia + 3% potassium chloride in 60% methanol.* S.P. = starting point. 1 = DNP-Gly; 2 = DNP-Ala; 3 = DNP-Ser; 4 = DNP-Thr; 5 = DNP-Val; 6 = DNP-Leu; 7 = DNP-Ile; 8 = DNP-Pro; 9 = DNP-Met-O_2; 10 = DNP-Trp; 11 = DNP-Phe; 12 = Di-DNP-Tyr; 13 = DNP-Asp; 14 = DNP-Glu; 15 = DNP-$CySO_3Na$; 16 = Di-DNP-Lys; 17 = α-N-DNP-Arg; 18 = Di-DNP-His; 19 = DNP-OH; 20 = DNP-NH_2. Reproduced from ref. 34 with permission.

3. DETECTION

The localization, characterization and identification of spots are essential aspects of TLC. The techniques used in two-dimensional TLC are identical with those used in one-dimensional TLC, except that the whole surface of the plate has to be scanned, which makes the problems much more difficult. Detection may therefore require a very long time and very sophisticated instrumentation, contrasting with the great simplicity of the separation method. Techniques for recovering or displaying the two-dimensional separation have benefitted from recent improvements in image processing made possible through the availability of powerful, yet cheap, computers.

In two-dimensional chromatography the exact position of the spot must be determined for qualitative analysis and the whole spot profile, in both directions, must be integrated for quantitative analysis. The problem is therefore much more difficult than in conventional TLC, where the centre of the spot is on the vertical of the sample spot and the solute concentration profile in the direction perpendicular to that of the development is devoid of interest and can be integrated at once, as is done with the use of a narrow slit perpendicular to the scanning direction in photodensitometers for TLC. Such devices cannot be used in two-dimensional TLC; the spatial resolution of the scanner, whether an optical beam, an electronic beam or any other system, must be small compared with the spot size, about 10–20 times smaller in dimension than the spot base width. Typically, this means that it should not exceed 0.1–0.5 mm in diameter, depending on the TLC conditions. If ω is the width of the sensor beam and L the development length, a number L/ω of parallel scans must be carried out. This number varies from about 100 to around 2000 depending on the conditions, but in any case is large. Convenient software must be available to align these scans, detect the spots and segment and integrate them.

In the following we review the various detection methods used in conventional TLC and discuss how they can be applied to the special problem of two-dimensional TLC.

A laborious detection technique consists in scraping off the parts of the adsorbent layer containing each spot of interest and extraction from the adsorbent or *in situ* elution of the spot. Although some commercial equipment is now available (for example, Eluchrom Automatic Elution System from Camag), which considerably reduces the amount of solvent necessary for recovering the sample, this technique is inconvenient, time consuming and not quantitative. A final measurement step must also be added, such as a spectrophotometric determination. To apply this method the spot must first be located precisely.

One-dimensional TLC has sometimes been coupled with gas detection devices: detection of compounds eluted on a Chromarod can be performed either with a flame-ionization detector[37] or by direct insertion into a thermoionic[38] or mass spectrometric[39] detector. However, these techniques are not suitable for two-dimensional TLC because of their lack of spatial resolution and/or the considerable amount of time necessary for the scans.

Spots may be revealed after performing adequate chemical tests. Reagents for these tests are often sprayed on the layer. The non-uniformity of the spray may drastically affect the detection of the linearity of response. Therefore, whenever possible spots are rendered visible by exposure to gaseous reagents, which act more uniformly.

Coloured or fluorescent spots can be easily detected visually under white or UV light. If the compound itself is not visible or fluorescent, detection can be performed by applying gaseous, colorimetric complexing agents or even radioactive markers, or by using the quenching effect of the compound on the fluorescence of an additive in the chromatographic bed. The compound then appears as a black spot on a brilliant background. This method permits the accurate determination of the position of the spot, but not of its size or concentration. The latter are determined by the use of one of the photometric methods of TLC classified as densitometric and fluorimetric techniques.

Densitometry can be carried out in the transmission or the reflection mode. It measures the intensity of the light transmitted through the TLC plate or reflected by it. Quantitation is based on the decrease in light transmitted or reflected by the spot in comparison with the neighbouring background[40]. It requires background suppression and assumes a relationship between the signal and the concentration of a compound. This relationship is linear only at very low concentrations[41]. For higher concentrations it is not given by the conventional Beer's law but by the Kubelka–Munk equation[40], because of diffusion of light by the particles in the layer. The response factor of a compound depends on its coefficients of light adsorption and scattering[40]. Obviously the densitometric measurements must be made using a monochromatic incident beam, and the wavelength must be optimized depending on the compounds of interest. Transmission densitometry has been shown theoretically[42] to be more sensitive than reflectometry, although layer uniformity is more critical in the former method. Both non-uniformity of the layer and poor light intensity affect the signal-to-noise ratio. However, such problems may be overcome to some extent with a double-beam instrument. Reflectometry is more widely used because of the higher

optical density of most compounds, especially in the UV range. Frei[40] published an extensive study on reflectance spectroscopy. Using double-beam instruments, one can also compensate for the background effects due to the layer.

In fluorimetry, the incident radiation excites the various compounds, and those which emit secondary radiation are detected. This emitted light is characterized by a longer wavelength than the incident radiation. The non-spotted, background or base regions of the layer do not fluoresce. The excitation wavelength can be adjusted to optimize the sensitivity of the measurement for a given compound. The most commonly used wavelengths are 254 and 360 nm.

Fluorescence measurements can also be carried out in the so-called quenching mode. A phosphor additive is mixed to the sorbent slurry before coating the plate. When the developed plate is irradiated with UV light the base regions of the plate emit a uniform visible light, while the sample compounds appear as dark spots. This method is more sensitive when the light is transmitted from the back of the plate.

Many commercially available instruments are single-wavelength devices in which a monochromatic beam is used to scan the plate surface. They can be applied to all modes of densitometry or fluorimetry, with the use of suitable mirrors and filters. In the fluorescence mode, better instruments permit the adjustment of both the excitation and emission wavelengths. In these instruments the scanning optical beam is supposed to illuminate on the plate a rectangle with a very large aspect ratio, the long dimension (*ca.* 1 cm) being perpendicular to the scanning direction. This yields a signal proportional to the light intensity perceived, *i.e.*, integrated over the whole slit length. If the relationship between light intensity and spot concentration is non-linear, this results in quantitative errors when the concentration is not constant along the slit. On the other hand, this permits integration of the fluctuations due to layer heterogeneity over a larger area and decreasing the noise. Hence, the signal should be integrated over the slit to linearize the characteristic response of a single slit in terms of concentration[43]. Knapstein *et al.*[44] obtained a linear calibration graph for steroids detected on silica gel in the quenching mode.

With dual-wavelength densitometers, fluctuation of the light source is balanced and a flying spot can replace a fixed slit aperture, which leads to greater accuracy in quantitation. The complexity of dual-wavelength densitometers requires computer-assisted processing of the signal[45]. Speed, like resolution, is expensive and rapid evaluation of a one-dimensional thin-layer chromatogram requires the scanner to be connected either to a recorder or to a video screen. Speed can also be achieved at the expense of a lower sensitivity if the signal noise depends on the integration time.

In 1976, Devenyi and co-workers[46,47] introduced video techniques in the densitometric evaluation of thin-layer chromatograms. The whole chromatogram is irradiated by a suitable light source of relatively homogeneous intensity and an image is taken by a Vidicon camera. This is extremely fast and also reasonably accurate and sensitive, and the rather sophisticated processing such as background subtraction or spot integration is easy to carry out in an interactive mode.

Generally, the HPTLC scanners available for photodensitometric measurements cannot be adapted easily to two-dimensional TLC. The speed of detection is an extremely critical factor as all of the plate surface has to be scanned. Scanning a conventional TLC plate takes a few minutes, but scanning a two-dimensional plate would take from several hours to one day. No software is available to align all these scans and process them to obtain quantitative information.

Two-dimensional detection devices have resulted mainly from two-dimensional gel electrophoretic analyses[48,49] and from the TLC of radioactive compounds[8]. In both instances an autoradiograph is obtained and then scanned with a very narrow visible light beam (spatial resolution around 0.1 mm or below). Complete data acquisition and processing systems have been developed by several groups[48–50]. These systems offer possibilities of data acquisition, filtering, background subtraction, calibration and data reduction, and provide for spot detection, segmentation, integration, pairing and data file handling on thousands of spots.

Video-densitometric techniques have been applied to two-dimensional TLC. A two-dimensional matrix of pixels has sometimes been used[47,51] together with a Vidicon camera to obtain both normal two-dimensional and spectral images. Both fluorescence and absorption measurements can be carried out with this technique. The sensitivity of this type of detector is in the nanomole range. Although its main drawbacks are cost and complexity, it is still more attractive to the analyst than the classical spectrodensitometer, the use of which is tedious and time consuming and necessitates image reconstitution after hundreds of one-dimensional scans of a two-dimensional plate.

Recently, Guiochon and co-workers[52,53] conceived the use of a detection device on-line with a two-dimensional liquid chromatographic system. Detection is now performed in the elution mode, in the second direction, with a photodiode array Reticon camera used as a series of individual UV cells parallel to the exit edge of the plate. In this system, the solvent is pumped through the chromatographic bed under pressure and no longer moves under the influence of capillary forces. At the exit, the solvent is forced through a slot which constitutes the detector cell.

A monochromatic light passes through this slot and is focused on the diode array of the Reticon camera. A time-dependent signal similar to the line signal of an autoradiography scan is recorded and processed through a data acquisition system, then displayed on a colour TV screen. HPLC elution conditions may thus be reproduced and quantitation is no longer affected by plate characteristics and chromatographic bed diffusivity as in regular TLC.

4. APPLICATIONS

The separations that have been accomplished using two-dimensional TLC are classified in this section under lipids, pigments, alkaloids, proteins and their constituents, carbohydrates, glycopeptides, nucleic acids and their constituents, environmental pollutants, pesticides and miscellaneous. We have tried to emphasize the peculiarities of various assays by analysing the chromatographic behaviour of solutes. The retention and chromatography of compounds may involve adsorption, partition, ion exchange or restricted diffusion (gel permeation). Although one particular chromatographic mechanism may be emphasized for the retention of solutes under given conditions, other concurrent processes should not be forgotten.

4.1. Lipids

"Lipids" is a term used to qualify various classes of compounds that are characterized in general by solubility in organic solvents and insolubility in water. In this

TABLE 1

SEPARATION OF FATTY ACIDS AND THEIR ESTERS

N is the number of spots resolved in the best published chromatogram. Compounds: name of classes, groups or individual compounds studied. Stationary phase: composition of the thin layer used as the chromatographic bed. Also includes dimensions and activation conditions when available. When two different phases are used, 1 refers to the phase used for the first development, usually a narrow strip along the edge of the plate, and 2 to the second stationary phase. SSP: sample spot position; distance from the edges of the plate. Solvent 1: composition of the solvent used for the first development. Sometimes several successive developments are carried out using different solvents. Their compositions are given in the order a, b, c, etc. *t/L*: time (min) or length (cm) of the first (with solvent 1) and second (with solvent 2) developments. Drying: conditions under which the plate is dried after the first development is finished. Solvent 2: same as solvent 1, but for the second development. Ref.: also includes figure numbers, if one is reproduced here.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
	Alkenyl acyl-, alkyl acyl- + diacyl glyceryl acetates	Si gel G, 110°C, 1 h		Skelly F–diethyl ether (88:12)	14 cm	N_2 dry	Toluene		54
11	Fatty acids, prostaglandins, thromboxanes	Si gel, 20 × 20 cm		Diethyl ether–CH_3OH–acetic acid (90:1:2)			Chloroform–methanol–acetic acid–water (90:8:1:0.8)		55
13	Fatty acids esters	Si gel D.B., Camag, 20 × 20 cm, 0.25 mm, wash, 139–142°C, 30 min	2.5	Light petroleum–diethyl ether–acetic acid (75:25:2.5)	70–80 min, 16 cm	15 min, room temp.	Diethyl ether–light petroleum–acetic acid (70:30:1)	65–75 min, 15 cm	56
8	Ginsenosides	Silanized Si gel 60 F254, 20 × 20 cm, 0.25 mm	2.0	(a) Chloroform–methanol–ethyl acetate–butanol–water (4:4:8:1:2) (b) Chloroform–butanol–methanol–water (4:8:3:4)	10 cm	air dry, 10 min	(c) Chloroform–methanol–water (13:7:2)	10 cm	57
13	Mercury(II) adducts of unsat. esters (mono-, di-, tri-, tetra-, penta-, hexa-enes)	(1) Si gel G–Kieselguhr (3:7), 20 × 20 cm (2) Impregnate with 10% paraffin in light petroleum		On (1): isobutanol–formic acid–water (8:8:5)	Top	1 h air, 10 min H_2S chamber	On (2): formic acid–acetonitrile–acetone (8:8:5)		58
16	Trialkylglyceryl esters, dialkoxyglycerides, alkoxyglycerides + *n*-glycerides	(1) Si gel G, 4 × 20 cm, 0.25 mm (2) $AgNO_3$-impregnated Si gel G, 16 × 20 cm, 0.25 mm. 110–120°C, 1–2 h	2.0	On (1): petroleum hydrocarbon–diethyl ether (90:10) (need 50% relative humidity)			On (2): petroleum hydrocarbon–diethyl ether (90:10) (2 ×) (need 50% rel. humidity)		59 (Fig. 3)
4	Positional isomers of hydrostearic acid	Si gel G, 0.25 mm		Benzene–acetone (20:1)			Benzene–acetone (20:1)		60

section, four main groups of substances are considered: fatty acids and their esters, steroids, phospholipids and glycolipids. The different two-directional assays are briefly discussed in the text and detailed chromatographic conditions are given in Tables 1–5.

4.1.1. Fatty acids and their esters (Table 1)

Separations of various glyceryl acetates[54] and of some fatty acids from prostaglandins and thromboxanes[55] have been achieved on silica plates owing to the different selectivity of the solvent system in each direction. Fatty acid esters have also been resolved on silica[56] with a more polar eluent in the second than in the first direction.

A special category of compounds, the ginsenosides (triterpenoid saponins of the dammarane type), have been assayed on silanized silica gel using a less polar mobile phase in the second than in the first direction[57].

El-Zeany and Ahmed[58] devised an original method to resolve fatty acid esters. They first separated the mercury(II) adducts of these unsaturated esters on a 3:7 silica gel–Kieselguhr adsorbent with isobutanol–formic acid–water, based on the different degree of solute unsaturation. Then, the plate was positioned in a hydrogen sulphide chamber; mercury(II) sulphide was deposited as black spots and the esters were liberated. Chromatography in the second direction was accomplished after impregnating the plate with paraffin. The esters partitioned between that phase and the formic acid–acetonitrile–acetone eluent. Their mobility was a function of chain length. Whereas is this method mercury(II) adducts of solutes were chosen to achieve separations based on different degrees of unsaturation, more commonly unsaturated compounds are resolved according to their ability to form coordination complexes with ions (such as silver) which impregnate the stationary phase. Schmid *et al.*[59], for instance, after separating glycerol esters into four classes according to basic structure, type and number of functional groups on plain silica gel, differentiated each class according to the number and configuration of the double bonds in the constituent compounds, on silica gel impregnated with silver nitrate (Fig. 3).

4.1.2. Steroids (Table 2)

This class of lipids, of which cholesterol is a common representative, includes physiologically important compounds such as the bile acids, the androgens and the oestrogens, and essential metabolic regulators, such as the adrenocortical hormones. Thus, the separation of these substances and their quantitation in biological samples are essential, especially for diagnostic purposes.

Using silica, Bouillé *et al.*[61] first eluted the impurities associated with cortisone in plasma and adrenal extracts. Chromatography in the orthogonal direction was achieved with a more polar mobile phase containing water, which resulted in the migration of corticosterone from its original position on the plate. Also using a silica phase, Bicknell and Gower[62] succeeded is resolving a mixture of polar and non-polar compounds. Two successive developments in the first direction with benzene–diethyl ether (9:1) permitted the separation of the non-polar C_{19} 16-unsaturated steroids 5α-androst-16-en-3β-ol, 5β-androst-16-en-3α-ol, 5α-androst-16-en-3α-ol, 1,3,5-[10],16-oestratetraen-3-ol and 5α-androst-16-en-3-one. The use of a more polar eluent, benzene–methanol (9:1), for development in the second direction permitted

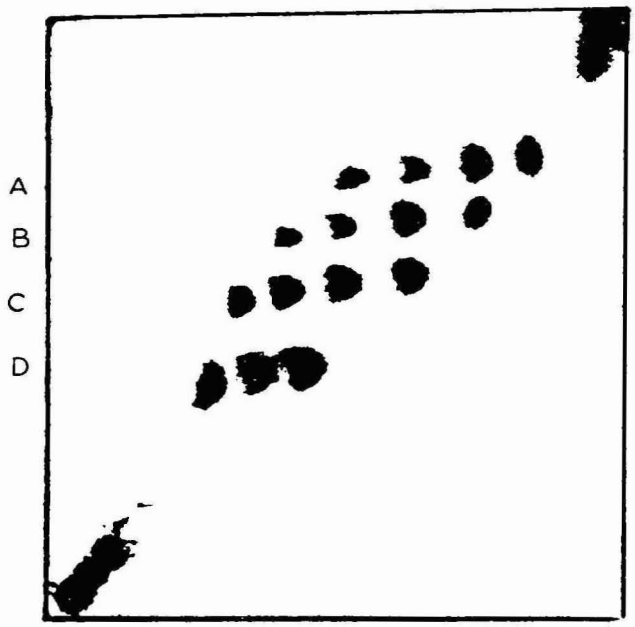


Fig. 3. Two-dimensional chromatogram of a model mixture containing the following compounds: (A) trialkyl glyceryl ethers: trioctadecyloxypropane, 1,2-dioctadecyloxy-3-octadecenyloxypropane, 1-octadecyloxy-2,3-dioctadecenyloxypropane, trioctadecenyloxypropane; (B) dialkoxyglycerides; 2,3-dioctadecyloxy-1-O-octadecanoylpropanol, 2,3-dioctadecyloxy-1-O-octadecenoylpropanol, 2,3-dioctadecenyloxy-1-O-octadecanoylpropanol; (C) alkoxydiglycerides; 3-octadecyloxy-1,2-di-O-octadecanoylpropanediol, 3-octadecenyloxy-1,2-di-O-octadecanoylpropanediol, 3-octadecyloxy-1,2-di-O-octadecenoylpropanediol, 3-octadecenyloxy-1,2-di-O-octadecenoylpropanediol; (D) triglycerides: tri-O-octadecanoylpropanetriol(tristearin), 1,2-di-O-octadecanoyl-3-O-octadecenoylpropanetriol (oledodistearin), 1-O-octadecanoyl-2,3-di-O-octadecenoylpropanetriol (stearodiolein), tri-O-octadecenoylpropanetriol (triolein). Solvents: first direction, petroleum hydrocarbon–diethyl ether (90:10), developed once on plain silica gel G strip; second direction, petroleum hydrocarbon–diethyl ether (90:10) developed twice on silver nitrate-impregnated silica gel G. Indicator: charring after spraying with chromic–sulphuric acid solution. Reproduced from ref. 59 with permission.

the separation of the more polar Δ^4-3-oxosteroids testosterone and progesterone and of the Δ^5-3β-hydroxysteroids pregnenolone and 5,16-androstadien-3β-ol.

Taylor[63] separated thirteen polar Δ^4-3-oxosteroids and oestrogens on silica with chloroform–methanol–water (94:6:0.5) in the first direction, followed by cyclohexane–ethyl acetate (50:50) in the second direction (Fig. 4). Cavina *et al.*[64] achieved similar resolutions of oestrogens and progestagens on silica by combining appropriate different developing systems. Clearly, the polarity of the mobile phase, its constituents and the degree of deactivation of the stationary phase achieved by use of water in the eluent are all factors that affect such assays.

Issaq[65] resolved two isomeric pairs, namely 7α- from 7β-hydroxycholesterol and 5β,6β- from 5α,6β-epoxycholesterol on a special plate with two different sorbents coated side-by-side. Chromatography in the first direction was accomplished on silica gel with diethyl ether as the eluent. Orthogonal elution was then achieved for a few centimetres on silica and, for the remaining part, on silanized silica, with a non-polar heptane–HMDS (98:2) as the mobile phase.

Similarly, Levitt and Touchstone[66] separated six bile acids on a two-phase plate where a 3 × 20 cm reversed-phase strip had been coated at the side of a 17 × 20 cm silica layer. Reversed-phase chromatography was carried out on the thin strip with an acid–organic eluent mixture and resulted in the separation of the bile acids into three classes: cholic, deoxycholic and chenodeoxycholic. Orthogonal development with the mixed aqueous (acetic acid–water) and organic (chloroform–methanol) solvent on the silica phase further separated the taurine from the glycine conjugates in all three classes of compounds. It is important to remember that these bile acids have functionalities that interact strongly with silica unless the adsorbent is modified through bonding with alkyl chains (reversed-phase strip) or deactivated by the presence, in the mobile phase, of components such as acetic acid or water, which compete strongly with the solute for the available adsorptive sites.

Vidrine and Nicholas[67] resolved two different lipid classes, *viz.*, steroids and unsaturated aliphatic hydrocarbons (terpenoids), on a mixed thin-layer plate coated with a slurry of silica, silanized silica and calcium sulphate. The eluent was relatively non-polar in the first direction, and retention could be attributed to adsorption. In the second direction, however, a more polar eluent was used, containing 25% of water. Under these conditions, a partition–adsorption mechanism is probably in effect.

Finally, Curtius and Müller[68] achieved an original, truly two-dimensional GC–TLC separation of a hormone mixture. The first dimension involved a separation on a GC column with a split effluent, 10% directed to a flame-ionization detector and 90% spotted on a TLC silica plate which moved linearly with time. The development of this plate with chloroform–ethanol (90:10) represented the second dimension and improved the resolution obtained with GC alone (Fig. 5). Clearly, the second separation is not especially helpful with the twelve components shown here, which are sufficiently well resolved by the GC step for quantitative analysis. It is, however, of greater use with more complex mixtures that cannot be resolved by GC but are resolved by the two-dimensional separation scheme.

4.1.3. Phospholipids (Tables 3 and 4)

This lipid class includes the phosphoglycerides and sphingolipids, all important membrane constituents. Chromatography of these compounds is often accomplished on silica gel, in its pure form or impregnated with either boric acid, ammonium sulphate, magnesium acetate, magnesium silicate or magnesium hydroxycarbonate.

In general, separations of phosphoglycerides (Table 3) require development of the plate with a water–organic eluent containing acetic acid in one direction and a base such as ammonia solution in the other [69–73]. Thus, the mobility of the molecules in each direction is affected by the differing degree of ionization, *i.e.*, the extent of amine protonation and phosphate and/or carboxyl dissociation, as well as by the competition of the acid or base in the mobile phase for adsorptive sites on the silica plate. Moreover, Jain and Subrahmanyam[74] have reported that appropriate amounts of ammonium sulphate in the stationary phase and acetic acid in the eluent are important for obtaining spots with no tailing and good resolution.

It is interesting that, on a phase containing boric acid[75], phosphatidylinositol, which has vicinal *cis*-hydroxyl groups in its sugar moiety, is retained the longest (Fig. 6). This may exemplify the selective affinity of boric acid for *cis*-diol compounds.

TABLE 2

SEPARATION OF STEROIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
	Corticosterone purification	Kieselgel GF 254 (Si), 20 × 20 cm, 0.4 mm	2.0	(a) *n*-Hexane-ethyl acetate (4:1) (b) Ethyl acetate–cyclohexane–toluene (10:10:1)	20–30 min, 10 cm 30 min 10 cm	room temp.	Ethyl-acetate-chloroform-water (90:10:1)	30 min, 10 cm	61
17	Δ^4-3-Oxosteroids, Δ^5-3β-hydroxysteroids, C_{19}-16-unsat. steroids	Kieselgel G (Merck), 20 × 20 cm, 0.5 mm	2.0	Benzene–diethyl ether (9:1) (2 ×)	16.8 cm		Benzene-methanol (9:1)	16.8 cm	62
13	Δ^4-3-Oxosteroids, oestrogens	Kieselgel GF 254, 20 × 20 cm, 0.5 mm		Chloroform–methanol–water (94:6:0.5)	14.4 cm from spot		Cyclohexane-ethyl acetate (50:50) (2 ×)	18 cm	63 (Fig. 4)
6 or 8	Estrogens, progestagens	Si gel 60 F_{254}, 20 × 20 cm, 0.25 mm	2.0	Toluene–95% ethanol (90:10)	18 cm	Air dry, 20 min, dark	Butyl acetate-light petroleum acetic acid (70:30:1)	~18 cm	64

4	7α-Hydroxycholesterol, 7β-hydroxycholesterol, 5β,6β-epoxycholesterol, 5α,6α-epoxycholesterol	(1) 20 × 20 cm Si gel (2) 10 cm dipped in HMDS, 100°C, 2 h	(1) Diethyl ether	13 cm	Dry	(2) Heptane–HMDS (48:2)	~17 cm	65
6	Bile acids	2-D plate, 20 × 20 cm, CS Multi K (Whatman) (1) 3 cm KC 18 strip (2) remainder, Si gel	(1) Ethanol–0.01 *M* KH_2PO_4 (pH 2.5) (1:1)		Dry	(2) Chloroform–methanol–acetic acid–water (75:25:5:5)		66
8	Cholesterol, lanosterol, dihydrolanosterol, oxidosqualene, geraniol, *trans,trans*-farnesol, *cis,trans*-farnesol	Si gel G–silanized Si gel H–$CaSo_4 \cdot \frac{1}{2} H_2O$ (50:43:7), 20 × 20 cm	Hexane–ethyl acetate (90:10)	45 min, 14 cm		*p*-Dioxane–water (75:25)	2 h	67
12	Male and female hormones	(1) GC column impregnated with 3% XE-60 (2) Kieselgel G	(1) N_2, 50 ml/min, 210 → 265°C		Spray plate with HCl, split trimethylsilyl-esters	(2) Dichloromethane–acetone (70:30) or chloroform–ethanol (90:10)		68 (Fig. 5)

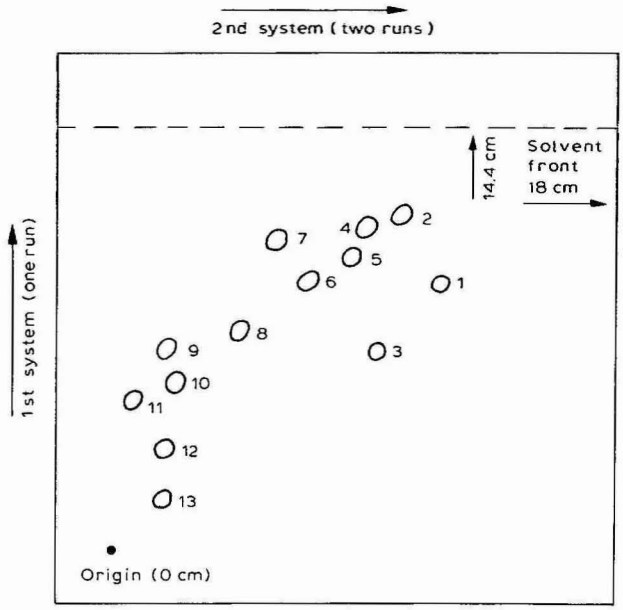


Fig. 4. Two-dimensional thin-layer chromatogram of steroids on silica gel. Solvent systems: (1) chloroform–methanol–water (94:6:0.5); (2) cyclohexane–ethyl acetate (50:50). 1 = Oestrone [3-hydroxy-1,3,5(10)-estradien-17-one]; 2 = progesterone(4-pregnene-3,20-dione); 3 = oestradiol [1,3,5(10)-estratriene-3,17β-diol]; 4 = androstenedione (4-androstene-3,17-dione); 5 = 17α-hydroxyprogesterone (17α-hydroxy-4-pregnene-3,20-dione); 6 = testosterone (17β-hydroxy-4-androsten-3-one); 7 = deoxycorticosterone (21-hydroxy-4-pregnene-3,20-dione); 8 = 11-deoxycortisol (17α,21-dihydroxy-4-pregnene-3,20-dione); 9 = corticosterone (11β,21-dihydroxy-4-pregnene-3,20-dione); 10 = cortisone (17α,21-dihydroxy-4-pregnene-3,11,20-trione); 11 = aldosterone (18,11-hemiacetal of 11β-21-dihydroxy-3,20-dioxo-4-pregnen-18-al); 12 = cortisol (11β,17α,21-trihydroxy-4-pregnene-3,20-dione); 13 = oestriol [1,3,5(10)-estratriene-3,16α,17β-triol]. Reproduced from ref. 63 with permission.

Pollet *et al.*[77] achieved the separation of different lipid classes, namely cholesterol, cerebrosides, sulphatides, phospholipids and gangliosides, on plain silica gel by repetitive elution with chloroform–methanol solutions of varying polarity in orthogonal directions (Table 4). Radwan[78] and Ikawa and Goto[79] resolved mixtures of fatty acids, steroids, phospholipids and other compounds on silica with an organic–acidic phase in one direction and an organic–basic phase in the other. Hubmann[80] was able to separate these various substances using different eluents for successive developments in each direction, owing to the different selectivity of each organic modifier with respect to the various solutes (Table 4).

4.1.4. Glycolipids (Table 5)

Glycolipids, such as the cerebrosides and the more complex gangliosides, are sugar-containing membrane lipids. The separation of such compounds was performed on silica gel by Ohashi[81], who used chloroform–methanol–aqueous ammonia to develop the plate in the first direction and *n*-propanol–aqueous ammonia in the second. Ledeen *et al.*[82], and subsequently Hunter *et al.*[83], in assaying for brain gangliosides, modified these conditions to a certain extent: ammonia was included in one dimension only, while salt was added to either or both solvents.

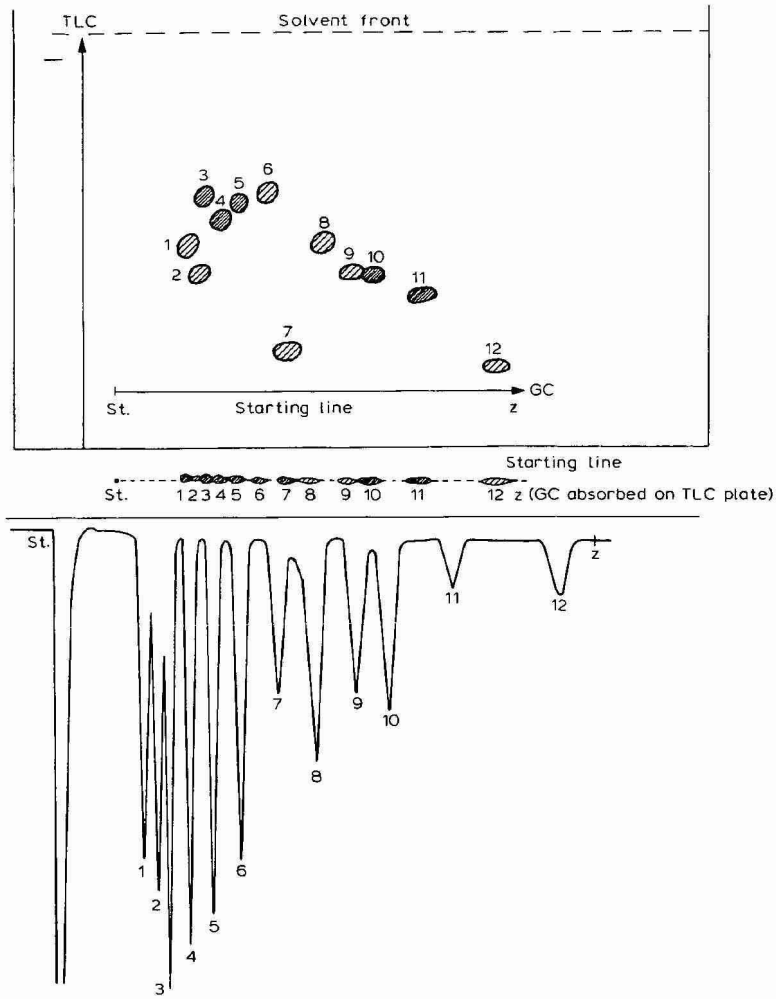


Fig. 5. Two-dimensional chromatography of twelve steroids (trimethylsilyl derivatives) using GC and TLC in combination. The lower part of the figure represents the gas chromatogram and the upper part illustrates the TLC separation after plate elution. It may be noticed that solutes 1, 2 and 3 are completely resolved after the TLC step. 1 = Allopregnandiol; 2 = pregrandiol; 3 = androsterone; 4 = etiocholanolone; 5 = dehydroepiandrosterone; 6 = pregnanolone; 7 = pregrantriol; 8 = 11-ketoandrosterone; 9 = 11-ketoetiocholanolone; 10 = 11-hydroxyandrosterone; 11 = 11-hydroxyetiocholanolone; 12 = pregnantriolone. St = starting point. Reproduced from ref. 68 with permission.

Cardenolides, which are glycosides with a steroid moiety, constitute a different category of sugar-containing lipids. Thirty-two cardenolides were separated by Clarke and Cobbs[84] on silica with a different solvent system for each direction. A correlation between the chromatographic mobility of the compounds and their chemical structure was observed. The number and position of the hydroxyl substituents played an important role in solute retention (Fig. 7).

TABLE 3

SEPARATION OF PHOSPHOLIPIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
6	Phosphatidyl (P) glycerol (G), pserine (PS), P-ethanolamine (PE), pinositol (PI), leathin (L), sphingomyelin (S)	Si gel H with 5% ammonium sulphate, 20 × 20 cm		Chloroform–methanol–water–gl. acetic acid (65:25:4:8)	10 cm	70°C, 5 min	THF–methylol–methanol–2 *M* ammonia (40:28.5:7.8:4.2)	10 cm	69
6	PG, PE, PI, PS, L, S (in amniotic fluid)	Si gel H with 50 g/l ammonium sulphate, 20 × 20 cm, 110°C, 30 min		Chlofororm–methanol–water–acetic acid, 17.4 *M* (162.5:65.0:10.0:0.5)	10 cm	70°C, 5 min	THF–methylol–methanol–2 *M* ammonia (120:80:35:10)	10 cm	70
13	PE, PC, PS, PI, L, S, and others, cerebrosides and sulphatides (in brain and mitochondrial inner membrane)	Si gel H (20 g) with magnesium acetate (1.5 g), 0.25 mm, N_2, 50% humidity, 30 min		Chloroform–methanol–28% aq. ammonia (65:25:5)		Dry, 10 min, N_2	Chloroform–acetone–methanol–acetic acid–water (3:4:1:1:0.5)		71

10	PI, PS, PE, PG, etc. (in erythrocytes)	Si gel with 1% alkaline magnesium silicate or 2% magnesium hydroxycarbonate		Chloroform–methanol–7 *M* ammonia (90:54:11)		Dry, 15 min; if rel. hum. >65%, dry 1 h *in vacuo*	Chloroform–methanol–acetic acid–water (90:40:12:1)			72
11	PI, PS, PG, etc. (in yeast)	Si gel H, 20 × 20 cm, 0.25 mm		Chloroform–methanol–acetic acid–water (52:20:7:3)	60–90 min	Air dry, 20 min, wash with diethyl ether, air dry, 20 min	Chloroform–methanol–40% aq. methylamine–water (13:7:1:1)			73
9	PG + derivatives, cardiolipin	Si gel G (25 g) with 0.4 *M* boric acid (50 ml), 20 × 20 cm, 0.25 mm, 120°C, 1 h		Chloroform–methanol–H_2O–conc. NH_3 (70:30:3:2)		Dry, 30 min, N_2	Chloroform–methanol–water (63:35:5)			75 (Fig. 6)
	L, S from PI, PS, PE, etc.	Si gel-impregnated glass-fibre sheets (ITLC type SG), 100°C, 30 min	2	Dichloromethane–ethanol–water (100:25:3)	6 cm, 3 min	Air dry, 5 min	Chloroform–methanol–ammonia (170:20:3)		4 cm, 2 min	76

TABLE 4

SEPARATION OF PHOSPHOLIPIDS AND OTHER LIPID CLASSES

Column headings as in Table 1.

N	*Compound*	*Stationary phase*	*SSP (cm)*	*Solvent 1**	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
11	Phospholipids, cerebrosides, sulphatide (plasma, liver, brain)	Si gel impregnated with ammonium sulphate, 20 × 20 cm; 0.5 mm, 110°C, 1 h		Chloroform–methanol–acetone–water (60:25:8:4)	Top	50°C, 5 min	Chloroform–methanol–acetic acid–water (50:35:8:1)	Top	74
11	Cholesterol, cerebrosides, gangliosides, phospholipids (cellular membranes)	Si gel HPTLC 60 F 254 (Merck), 10 × 10 cm	2	(a) Chloroform–methanol–water (70:30:4)	Top	Bench dryer, few min	(b) Chloroform–methanol (1:4)	2/3 of the plate	77
				(d) Chloroform–methanol (2:1)		Bench dryer, few min	(c) Chloroform–methanol (2:1)	Up to the top	
17	Triglycerides, fatty acids, steroids, phospholipids (plant leaves)	Si gel H, 20 × 20 cm, 0.3 mm		Chloroform–methanol 7 *N* ammonia (65:30:4)			Chloroform–methanol–acetic acid–water (85:10:10:2)		78
17	Triglycerides, fatty acids, steroids, phospholipids (plant leaves)	Si gel H impregnated with 2% aq. ammonium sulphate, 20 × 20 cm, 0.3 mm, 110°C, 1 h		Acetone–benzene–water (91:30:8)			Chloroform–methanol–acetic acid–water (85:10:10:2)		78
15	Bile acids and salts, fatty acids, sterols, phospholipids (gall bladder)	Kieselgel H (type 60), 20 × 20 cm, 0.25 mm, 120°C, 1 h	1.5	Chloroform–ethanol–28% aq. ammonia (25:35:1)	15 cm	Air stream, 30 min	Chloroform–ethanol–ethyl acetate–acetic acid–water (8:6:5:4:1)		79
11	Fatty acids, triglycerides, steroids, phospholipids (serum)	Si gel, 4.5 × 2.6 cm		(a) Chloroform–methanol–water (65:25:4)	3 cm		(c) *n*-Hexane–diethyl ether–gl. acetic acid (85:20:2) (for lower right-hand side of plate)	2.6 cm	80
				(b) *n*-Hexane–diethyl ether–gl. acetic acid (85:20:2)	4.5 cm		(d) Butanol–gl. acetic acid–water (60:20:20)	2.6 cm	

* (a), (b), (c), (d) indicate the sequence of developments.

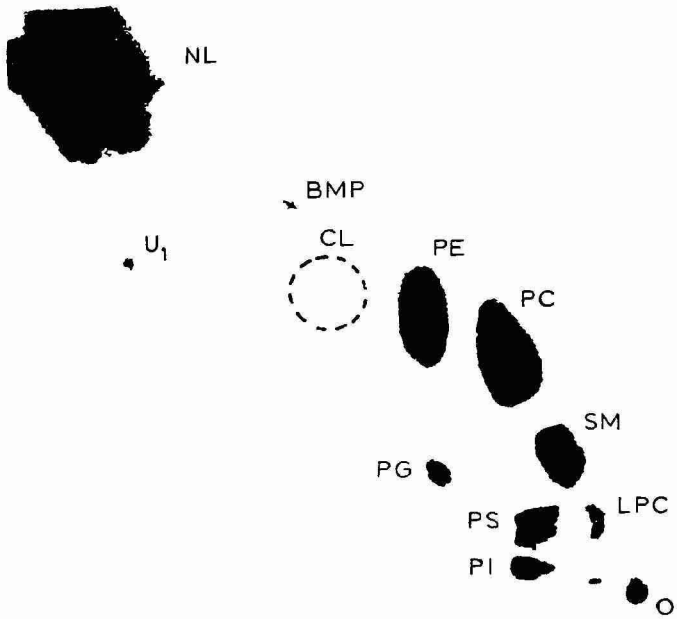


Fig. 6. Two-dimensional thin-layer chromatogram of rat lung liquids on silica gel impregnated with boric acid. Abbreviations: NL = neutral lipids; UI, unidentified; BMP, bis(monoacylglyceryl)phosphate; CL = cardiolipin; PE = phosphatidylethanolamine; PC = phosphatidylcholine; PG = phosphatidylglycerol; SM = sphingomyelin; PS = phosphatidylserine; PI = phosphatidylinositol; LPC = lysophosphatidylcholine; O = orgin. The solvent for development in the vertical direction was chloroform–methanol–water-concentrated ammonia (70:30:3:2) and in the horizontal direction chloroform–methanol–water (65:35:5). Reproduced from ref. 75 with permission.

4.2. Pigments

This general group contains the various carotenes, xanthophylls, porphyrins and anthocyanidins, *i.e.*, all natural pigments, and the synthetic tannins. Detailed conditions for their two-dimensional separation are reported in Table 6.

Xanthophylls were chromatographed by Knowles and Livingston[86] on a 1:4 magnesium oxide–Celite strip in the first direction and a 1:6 silica gel G–calcium hydroxide layer in the second. Adsorbability increased with the number of hydroxyl groups on the cyclic moieties of the solutes, the presence of epoxide functionalities especially at the 5,8-position and the length of the conjugated double bond system (Fig. 8). Other separations of carotenoids have been achieved by Tirimanna[87] and Sherma and Zweig[88] The hydrocarbonaceous carotenes exhibited the largest R_F values on silica. Owing to its greater number of conjugated double bonds, zeaxanthin was more retained than lutein[87].

Porphyrin methyl esters were resolved by Elder[89] on a silica gel plate. A quaternary solvent system was used in the first direction. Retention was increased by carboxylic acid substituents at positions 2 and 4 of the porphyrin ring, as witnessed by the smaller R_F for coporphyrin in comparison with mesoporphyrin. Additional ethanoic acid substituents at positions 1, 3 and 5, as in uroporphyrin, further enhanced the adsorption interactions of the solute with the stationary phase. Of all the

TABLE 5

SEPARATION OF GLYCOLIPIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
	Gangliosides (rabbit brain)	Si gel 60, 20 × 20 cm, 0.25 mm		Chloroform–methanol–0.2% aq. $CaCl_2$ (50:40:10) or Chloroform–methanol–0.25% aq. KCl (50:40:10)	4 h		Chloroform–methanol–25 *M* aq. ammonia (50:40:10) or Chloroform–methanol–0.25% KCl in aq. ammonia (50:40:10)	5 h	82
11	Gangliosides (tissues)	Si gel (Merck), 10 × 10 cm		Chloroform–methanol–28% aq. ammonia–water (2 ×)		Over P_2O_5, 2 h, *in vacuo*	*n*-Propanol–28% aq. ammonia–water (75:5:25) or chloroform–methanol water (60:40:9)		81
32	Cardenolides (leaf)	Kieselgel 60 DC Fertigplatten, 20 × 20 cm, 0.25 mm	2	Ethyl acetate–dichloromethane–methanol–water (120:72:7:4)	2 h	Air	Dichloromethane methanol (9:1)	2 h	84 (Fig. 7)
	Sterioside (leaf diterpene glycoside) purification	Kieselgel G type 60 impregnated with boric acid, 20 × 20 cm, 0.5 mm		*n*-Butanol–ethyl acetate–isopropanol–water (35:100:60:30)			Ethyl acetate–acetic acid–water (8:4:1)		85

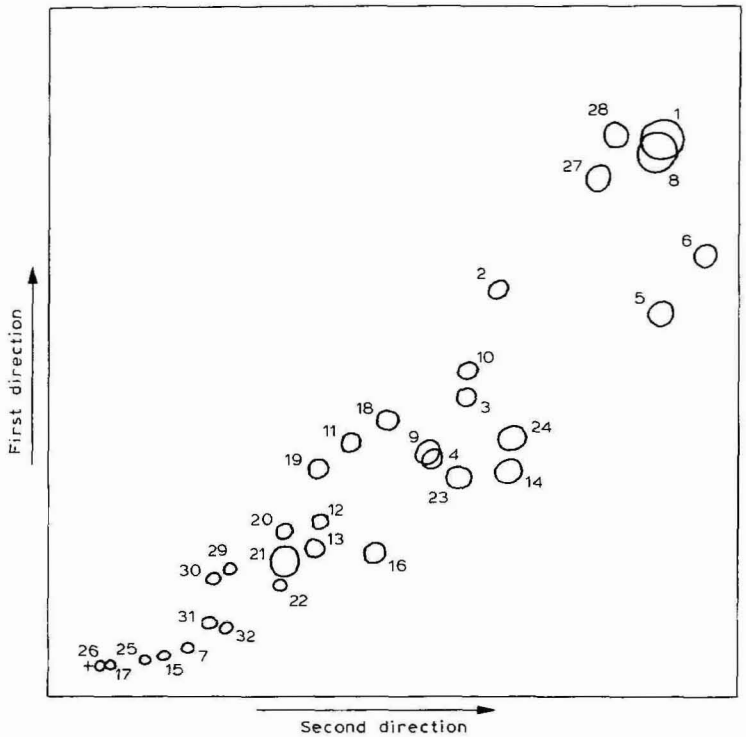


Fig. 7. Chromatogram of a mixture of cardesolide standards on silica gel. 1 = Digitoxigenin; 2 = digitoxigenin monodigitoxoside; 3 = digitoxigenin bisdigitoxoside; 4 = digitoxin; 5 = α-acetyldigitoxin; 6 = β-acetyldigitoxin; 7 = lanotoside A; 8 = gitaloxigenin; 9 = gitaloxin; 10 = gitoxigenin; 11 = gitoxigenin monodigitoxoside; 12 = gitoxigenin bisdigitoxoside; 13 = gitoxin; 14 = β-acetylgitoxin; 15 = lanatoside B; 16 = strospeside; 17 = digitalinum verum; 18 = digoxigenin; 19 = digoxigenin monodigitoxoside; 20 = digoxigenin bisdigitoxoside; 21 = digoxin; 22 = digoxoside; 23 = α-acetyldigoxin; 24 = β-acetyldigoxin; 25 = lanatoside C; 26 = deacetyl lanatoside C; 27 = α-anhydrodigoxigenin; 28 = β-anhydrodigoxigenin; 29 = diginatigenin; 30 = diginatigenin monodigitoxoside; 31 = diginatigenin bisdigitoxoside; 32 = diginatin. Solvent in the first direction, ethyl acetate–dichloromethane–methanol–water (120:72:7:4), and in the second direction dichloromethane–methanol (9:1). Reproduced from ref. 84 with permission.

compounds studied, haematoporphyrin was the only porphyrin with two hydroxyl groups and it was retained the most on the silica plate (Fig. 9).

Saitoh *et al.*[90] achieved the separation of various metal tetraphenylporphyrin chelates on a reversed-phase plate. The first development was carried out with acetone–propylene carbonate (20:80) and the second with acetone alone. Retention may be related to the ratio of the central metal electronegativity to its ionic radius, En/r_i[91]. Larger En/r_i values correspond to more delocalized chelate–metal bonds and smaller R_F values on the reversed-phase plate. In addition, chromatographic behaviour is affected by the configuration of each complex, whether planar, pyramidal or distorted octahedral, and its stability in each of the eluents used.

Anthocyanidins were resolved on cellulose by Mullick[92]. A methanol–acid–water solvent mixture did not differentiate between the methoxy and hydroxy group substituents on the anthocyanidin aromatic ring. A formic acid–hydrochloric acid or

TABLE 6

SEPARATION OF PIGMENTS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Dryuing*	*Solvent 2*	*t/L*	*Ref.*
14	Xanthophylls	(1) MgO–Celite (1:4) stripe (2) Si gel G–Ca(OH)$_2$ (1:6) layer	2.5 cm from end of MgO–Celite stripe	On (1): hexane–acetone (7:3) + ethoxyquin	40 min	Dry dark, 1–2 min, N_2	On (2): 2% butanol in benzene + ethoxyquin	1 h 20 min	86 (Fig. 8)
17	Carotenes, xanthophylls (seeds)	Si gel G, 0.35 mm, 100°C, 30 min		Chloroform–ethyl acetate (40:10)			Diethyl ether		87
7	Carotene, xanthophylls, chlorophyll	Si gel sheets, Eastman K 301 R, 15 × 15 cm		Benzene–acetone (3:1)	Top		Isooctane–acetone–diethyl ether (3:1:1)	Top	88
7	Carotene, xanthophylls, chlorophyll	Cellulose sheets		1% *n*-propanol in light petroleum			Light petroleum–benzene–chloroform–acetone–isopropanol (50:35:10:5:0.17)		88
11	Porphyrin methyl esters	Si gel, Camag D 5, 20 × 20 cm, 0.3 mm, dry at 110°C, 18 h exposure to air	3	Carbon tetrachloride–dichloromethane–methyl acetate–methyl propionate (2:2:1:1)	Top		(a) Benzene–butanone (40:3) (b) Chloroform–kerosene–ethanol (200:100:17)	Top Top	89 (Fig. 9)
7	Metal tetraphenylporphyrin chelates	RP-18 F 254s (Merck), 10 × 10 cm, 0.2 mm, 1 h at 110°C, cool in desiccator	1.5	Acetone–propylene carbonate (20:80) (2×)	7.5 cm		Acetone	7.5 cm	90
6	Anthocyanidins	Microcrystalline cellulose, Avicel SF, 20 × 20 cm, 0.25 mm		Formic acid–4 *N* HCl (2:1)	4.5 h		Methanol–conc. HCl–water (190:1:10)	2 h	92
6	Anthocyanidins	Microcrystalline cellulose, Avicel SF, 20 × 20 cm, 0.25 mm		Methanol–conc. HCl–water (190:1:10)	2 h		*n*-Amyl alcohol–acetic acid–water (2:1:1)	8 h	92
29	Tannin A or B constituents	Silica (Merck) GF 254, 110°C, 30 min		*n*-Butanol–acetic acid–water (4:1:5)	2 h, 15 cm		*n*-Butanol–ethanol–ammonia–water (75:10:15:10)	1.5 h, 15 cm	93

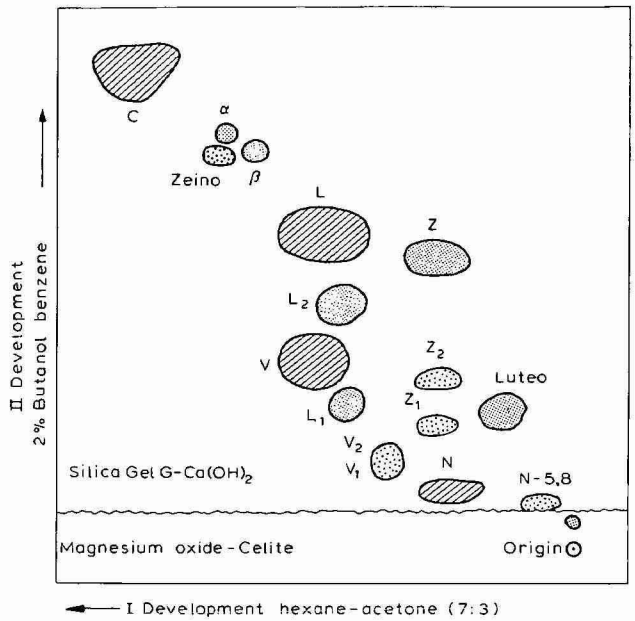


Fig. 8. Two-dimensional, two-adsorbent TLC of a carotenoid mixture on a magnesium oxide–Celite + silica gel G–$Ca(OH)_2$ plate. C = Carotenes; α = α-cryptoxanthin; β = β-cryptoxanthin; Zeino = zeinoxanthin; L = lutein; Z = zeaxanthin; L_1 and L_2 = lutein *cis*-isomers (corresponding to "neo-A" or "V" and "neo-B" or "U", respectively); V = violaxanthin; V_1 and V_2 = violaxanthin *cis*-isomers; Z_1 and Z_2 = zeaxanthin *cis*-isomers; Luteo = luteoxanthin; N = neoxanthin; N-5,8 = neoxanthin 5,8-epoxide. The first elution is on the magnesium oxide–Celite strip using hexane-acetone (7:3) and the second is on silica gel G–$Ca(OH)_2$ with 2% butanol in benzene. Reproduced from ref. 86 with permission.

amyl alcohol–acetic acid–water eluent used orthogonally did provide such a differentiation, and the retention increased with the number of hydroxyl substituents on the solute phenyl ring.

Finally, 29 intermediates in the synthesis of tannin A or B were separated on silica using an inorganic–acidic solvent mixture in one direction and an organic–basic eluent in the other. The migration sequence under alkaline conditions corresponded to different degrees of solute condensation or methylation whereas that under acidic conditions depended on the nature of the product[93].

4.3. Alkaloids

Heterogeneous nitrogenous substances produced by plants have been grouped under this heading. The two-dimensional chromatography of alkaloids pertaining to the cocaine, harmane, ergot and other families is considered here (Table 7).

Early attempts to separate opium[94], *Strychnos* and curare[95] alkaloids by two-directional paper chromatography were time consuming; development in one direction alone could require as long as 17 h.

TLC enabled faster analyses to be achieved. Using a silica gel plate, Munier and Meunier[96] separated seven cocaine alkaloids. Elution with a non-aqueous neutral mobile phase was followed by an orthogonal development in an acidic solvent

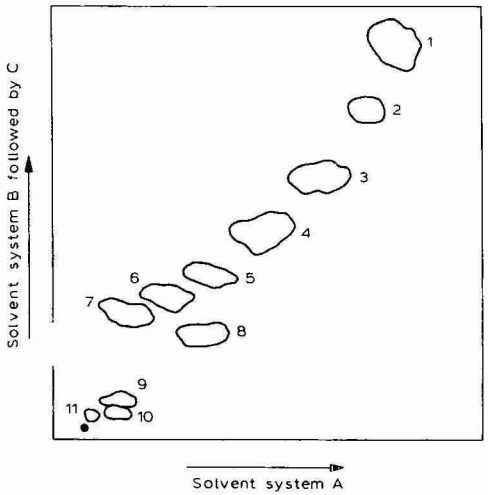
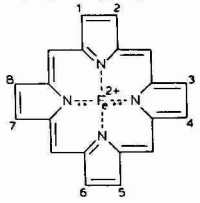


Fig. 9. Separation of a mixture of porphyrin methyl esters on silica by two-dimensional TLC. 1 = Mesoporphyrin IX; 2 = harderoporphyrin; 3 = coproporphyrin; 4,5,6 = penta-, hexa- and heptacarboxylic porphyrins, respectively; 7 = uroporphyrin; 8 = mono-β-hydroxypropionic monopropionic deuteroporphyrin IX; 9 = bis-β-hydroxypropionic deuteroporphyrin IX; 10 = haematoporphyrin IX; II = isohaematoporphyrin IX (all as their methyl esters). Basic structure:



No.	*Compound*	*Substituent in position*							
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*
1	Mesoporphyrin	CH_3	C_2H_5	CH_3	C_2H_5	CH_3	$(CH_2)_2COOH$	$(CH_2)_2COOH$	CH_3
3	Coproporphyrin	CH_3	$(CH_2)_2COOH$	CH_3	$(CH_2)_2COOH$	CH_3	$(CH_2)_2COOH$	$(CH_2)_2COOH$	CH_3
7	Uroporphyrin	CH_2COOH	$(CH_2)_2COOH$	CH_2COOH	$(CH_2)_2COOH$	CH_2COOH	$(CH_2)_2COOH$	$(CH_2)_2COOH$	CH_3
10	Haematoporphyrin	CH_3	$CH(OH)CH_3$	CH_3	$CH(OH)CH_3$	CH_3	$(CH_2)_2COOH$	$(CH_2)_2COOH$	CH_3

Solvent system for the first direction: (A) carbon tetrachloride–dichloromethane–methyl acetate–methyl propionate (2:2:1:1). Solvent systems for the second direction: (B) benzene–butanone (40:3) followed by (C) chloroform–kerosene–methanol (200:100:7). Reproduced from ref. 89 with permission.

TABLE 7

SEPARATION OF ALKALOIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
11	Major opium alkaloids	Acid-buffered Whatman paper No. 1 immersed in 2% ammonium sulphate, 28 × 32 cm, 0.3 mm	2.5	Isobutanol–glacial acetic acid (100:20)–water to saturation	16–17 h		90 ml of diethyl ether saturated with aq. phase (water or 0.1 *M* acetic acid)	2 h	94
7	Cocaine alkaloids (similar polarity and structure)	Si gel 60 (Merck), 20 × 20 cm, 0.25 mm	2.5	Methanol–carbon tetrachloride (50:50)	155 min		Acetone–acetic acid–water (72:8:20)	180 min	96
5	Alkaloids of unequal polarity and structure, morphine, codeine, thebaine, etc.	Si gel 60 (Merck), 20 × 20 cm, 0.25 mm	2.5	Ethyl acetate–2-nitropropane (50:50)	90 min		Methanol–carbon tetrachloride (50:50)	138 min	96
19	Morphine, codeine and derivatives	Activated Si gel G, 20 × 20 cm, 0.25 mm	1.5	Methanol–chloroform–ammonia (85:15:0.7)	15 cm	Air, 10 min	Hydrated diethyl ether–acetone–diethylamine (85:8:7)	15 cm	97 (Fig. 10)
13	Harmane alkaloids	Si gel 60 (Merck), 20 × 20 cm, 0.25 mm	2.5	Methyl ethyl ketone	98 min		Chloroform–methanol–acetic acid (64:16:20)	185 min	96
15	Alkaloids from *Rauwolfia corynantha*, pseudocinchona	Si gel 60 (Merck), 20 × 20 cm, 0.25 mm		Diisopropyl ether–methanol (85:15)	101 min	Dark, 30 min, 220°C	Acetone–acetic acid (90:10)	74 min	98
37	Ergot alkaloids	Si gel G, 20 × 20 cm, 0.25 mm, 110°C, 30 min	1.5	Methanol–chloroform (2:8)	15 cm	Air, 5 min	Diethylamine–chloroform (1:9)	15 cm	99
10	Ergot alkaloids	Si gel G in high-voltage electrophoresis apparatus, 20 × 20 cm, 0.25 mm	5 cm from anode, 4 cm from bottom edge	Acetic acid–pyridine buffer (pH 5.6), 1500 V, 45 mA	45 min	Fan dry, few minutes	Diethylamine–chloroform (1:9)		99 (Fig. 11)

containing 20% of water. Retention involved adsorption under the former conditions and a mixed partition–adsorption mechanism under the latter. The mobility of each cocaine alkaloid was approximately inversely proportional to the number of functional groups that can be adsorbed simultaneously on the silica gel, and also to the strength of adsorption of each group. Ecgonine, for instance, the only alkaloid in the mixture assayed to possess two strongly adsorptive groups (hydroxyl and carbonyl), on the same side of the six-membered ring, also exhibited the smallest R_F in both directions. Pseudococaine (2α-carbomethoxy-3β-benzoxytropane), with its adsorptive functionalities in different planes although on the same side of the ring, was less retained than cocaine (2β-carbomethoxy-3β-benzoxytropane), where both substituents are co-planar in the β-position.

Munier and Meunier[96] also achieved the separation of morphine, codeine, thebaine, narcotine and papaverine, alkaloids of different polarity and structure, on a silica gel plate developed with a weakly polar solvent in one direction and a more polar one in the other. Earlier work by Viala and Estadieu[97] involved the resolution of morphine, codeine and their derivatives by chromatography on activated silica. The first elution with methanol–chloroform–ammonia resulted in three spots, the most retained containing both morphine and codeine, the next corresponding to

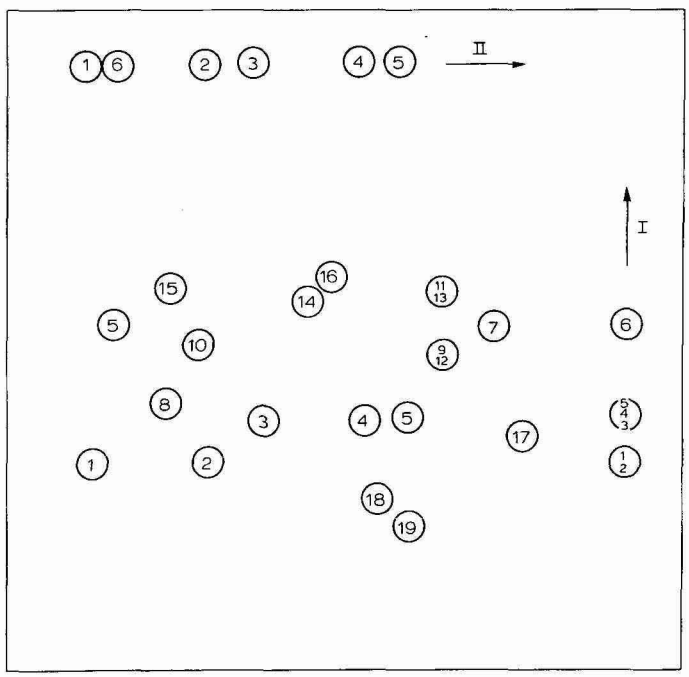


Fig. 10. Two-dimensional separation of morphine, codeine and their derivatives on silica. 1 = Morphine; 2 = codeine; 3 = O^6-monoacetylmorphine; 4 = diacetylmorphine; 5 = acetylcodeine; 6 = nalorphine; 7 = cocaine; 8 = quinine; 9 = nicotine; 10 = cotinine; 11 = methaqualone; 12 = diphenhydramine; 13 = mecloqualone; 14 = hydrochlorobenzethylamine; 15 = N-dimethyldiazepam; 16 = oxazepam; 17 = methadone; 18 = amphetamine; 19 = methylamphetamine. Solvent in the first direction: methanol–chloroform–ammonia (85:15:0.7), and in the second direction: hydrated diethyl ether–acetone–diethylamine (85:8:7). Reproduced from ref. 97 with permission.

heroin and the least retained to O^6-monoacetylmorphine and acetylcodeine. Orthogonal development in a mixture of hydrated diethyl ether, acetone and diethylamine differentiated all solutes (Fig. 10).

Harmane alkaloids[96] and alkaloids from *Rauwolfia, Corynantha* and *Pseudocinchona*[98] were resolved on silica using a polar neutral mobile phase in the first direction and a more polar, acidic solvent mixture orthogonally. Other than the nature of the solvent itself, which selectively affects the retention order, the pH of the eluent, which determines the ionization state of the molecule as a function of its pK_a value(s), also influences the retention behaviour. Whereas the first development of the silica plate in a neutral solvent did not resolve harmane from norharmane[96], the subsequent development in the acidic eluent provided such a differentiation; nor-

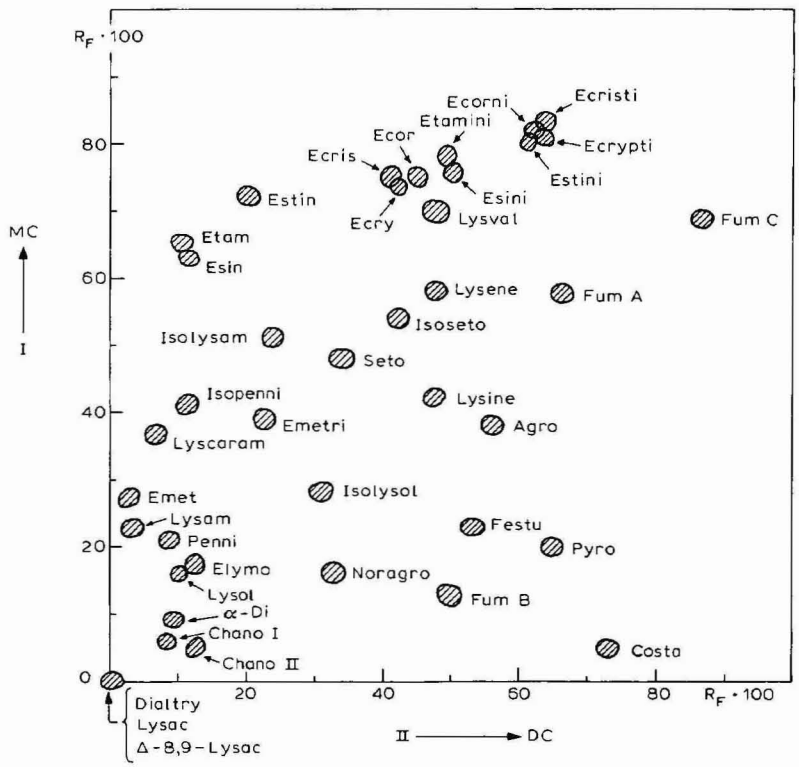


Fig. 11. Two-dimensional chromatogram of ergot alkaloids separated on silica gel G. Solvents: in direction I, MC = methanol-chloroform (2:8); in direction II, DC = diethylamine-chloroform (1:9). Agro = agroclavine; Chano I = Chanoclavine-(I); Chano II = chanoclavine-(II); Costa = costaclavine; α-Di = α-dihydrolysergol; Dialtry = DL-4-dimethylallyltryptophan; Elymo = elymoclavine; Ecor = Ergocornine; Econi = ergocorninine; Ecris = ergocristine; Ecristi = ergocristinine; Ecry = ergocrytpine; Ecrypti = ergocryptinine; Emet = ergometrine; Emetri = ergometrinine; Esin = ergosine; Esini = ergosinine; Estin = ergostine; Estini = ergostinine; Etam = ergotamine; Etamini = ergotaminine; Festu = festuclavine; Fum A = fumigaclavine A; Fum B = fumigaclavine B; Fum C = fumagaclavine C, Δ-8,9-Lysac = 6-methyl-$\Delta^{8,9}$-ergolene-8-carboxylic acid; Lysene = lysergene; Lysac = D-lysergic acid; Lysam = D-lysergic acid amide; Isolysam = D-isolysergic acid amide; Lyscaram = D-lysergic acid methylcarbinolamide; Lysine = Lysergine; Lysol = lysergol; Isolysol = isolysergol; Lysval = D-lysergyl-L-valine-methylester; Noragro = noragroclavine; Penni = penniclavine; Isopenni = isopenniclavine; Pyro = pyroclavine; Seto = setoclavine, Isoseto = isosetoclavine. Reproduced from ref. 99 with permission.

TABLE 8

SEPARATION OF AMINO ACIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
13	Cystine, serine, glycine, threonine, alanine, lycosine, valine, phenylalanine, arginine, etc.	Filter-paper sheet, 18 × 22 in.		Collidine	48–72 h		Water-sat. phenol, in atmosphere containing NH_3		3,100
19	Amino acids	Zeokarb 225 (WR 1.5–2.0) equilibrated with 0.2 *M* (pH 3.1) buffer		0.2 *M* buffer (pH 3.1)	1 day		*m*-Cresol–0.3% ammonia, + over ammonia vapor		102 (Fig. 12)
17	Amino acids	Whatman No. 3 MM filter-paper, 7 × 6 in.	1.5 cm from long paper edge, 4.5 cm from anode	Glacial acetic–formic acid buffer (pH 1.85), 20 kV, 100 mA	7 min	Dry, air, 40°C	2,4/2,5-Lutidine–ethanol–water (11:4:5)	2.5 h	103
18	Amino acids	Whatman No. 3 MM filter paper, 48 × 48 cm		Glacial acetic acid–formic acid, 21. kV (pH 1.85)	70 min	Warm air	*n*-Butanol–acetic acid water (4:1:5)	16 h	104
20	Amino acids (protein hydrolysate)	Microcrystalline cellulose, Avicel, 20 × 20 cm, 0.5 mm, room temp., 24 h	1.5	1-Butanol–acetic acid–water (3:1:1)	12 cm, 1.5 h	Air dry, room temp., 6 h	Phenol-water (3:1)	12 cm, 2 h	105
12	Amino acids (protein hydrolysate)	Cellulose ECS 6064, 10 × 10 cm, 100°C, 30 min, cool, wash with solvent 1, dry, room temp.	1.5	Methanol–water–pyridine (4:1:2)	25–30 min	Air, ambient temp.	Ethanol–1-butanol–water–propionic acid (5:5:2.5:1)	40-45 min	106

17	Amino acids (urine)	Cellulose + 2 cm ion exchange zone (desalting described)	On ion exchange zone	Pyridine–dioxane–NH_3–H_2O (35:35:15:15) (2 ×)	90 min		*n*-Butanol–acetone–acetic acid–water (35:35:10:20) (2 ×)	60 min	107
26	Polar + non-polar, natural + modified	Cellulose, short fibres, 20 × 20 cm, 0.25 cm		Propanol–formic acid–water (75:5:20)	~20 cm		Methyl ethyl ketone–2-methylpyridine–formic acid–water (31:47:2:20)	16 cm	110 (Fig. 13)
13	Bacterial cell-wall amino acids	Cellulose (Merck), 20 × 20 cm	1.5	Isopropanol–acetic acid–water (75:10:15)	3 h, 15.5 cm	Overnight, room temp., or rapid, 105°C	Methanol–pyridine–10 *N* HCl–water (64:8:2:14)	1.25 h, 15.5 cm	111
10	Amino acids	Si gel G (Merck), 20 × 20 cm, 0.35 mm		*n*-Propanol–34% ammonia (67:33)	18 cm	60°C, 30 min	0.2% ninhydrin in *n*-propanol–water glacial acetic acid (64:36:20)	18 cm	112
22	(Not all resolved) amino acids	Silufol (Kavalier), 15 × 15 cm	2	Ethyl acetate–isopropanol–water–ammonia (20:20:25:1.5)	13 cm	Air, 10 min; 110°C, 10 min; air, 10 min	Acetone–water–acetic acid–formic acid (50:15:12:3)	13 cm	113
36	Amino acids	Cellulose, 20 × 20 cm	2.5	*n*-Butanol–acetone–diethylamine–water (10:10:2:5) (pH 12)	Top		Isopropanol–formic acid–water (40:2:10) (pH 2.5)		115
13	Amino acids	Kieselgel G, 20 × 20 cm		2 *N* acetic acid–0.6 *N* formic acid buffer (1:1), pH 2, 460 V, 12.6 mA	1 h		*n*-Butanol–glacial acetic acid–water (3:1:1)		114

harmane, with the larger pK_a value, exhibited a higher chromatographic mobility.

Finally, ergot alkaloids were separated on activated silica gel after elution with chloroform–methanol in one direction, followed by an organic solvent–diethylamine in the orthogonal direction (Fig. 11). The strong diethylamine base helped to desorb the alkaloids by competing for adsorption on to silanols[99]. Agurell[99] also resolved nine ergot alkaloids on silica by combining thin-layer electrophoresis in one direction with chromatography in the other.

4.4. Proteins and their constituents

The two-dimensional chromatographic assays of amino acids, peptides and proteins, important morphological and physiological cellular components, are discussed here. Conditions for their separation are given in Tables 8–10.

4.4.1. Amino acids (Table 8)

Early reports by Consden *et al.*[3] and Martin and Synge[100] described the bidirectional separation of several amino acids on paper. The chromatographic behaviour of the solutes was found to be a function of their partition between the mobile phase and the water-saturated cellulose. The analysis time was extremely long, one elution alone requiring 2–3 days. After the pioneering studies of Cohn on ion exchange[101], slightly faster separations of amino acids were achieved on sulphonated polystyrene resin-loaded paper, for instance[102]. In the assay reported by Knight[102], the first eluent was a 0.2 *M* buffer at a pH of 3.1 and cation exchange determined the elution order: compounds such as lysine, arginine, ornithine, histidine, tryptopan, cysteine, tyrosine and phenylalanine, which contain two amine groups, each proton-

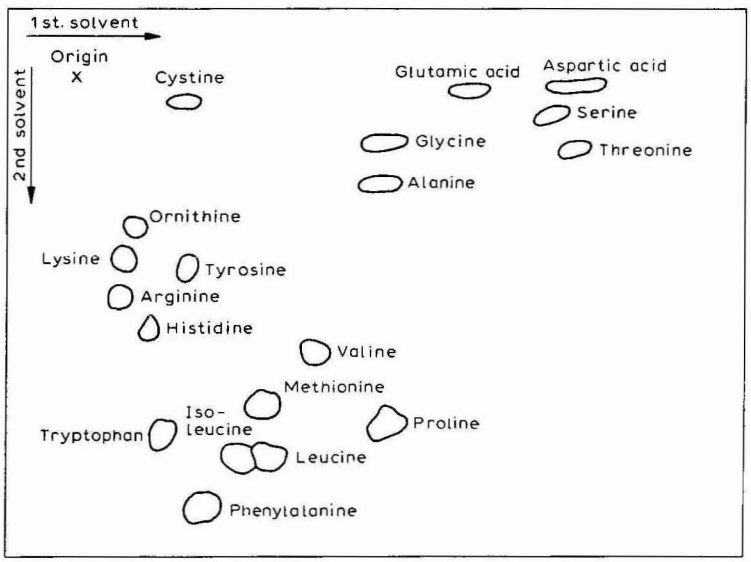


Fig. 12. Two-dimensional separation of amino acids on cellulose. Solvent used for the first development, 0.2 *M* buffer (pH 3.1), and for the second development, 0.3% ammonia in *m*-cresol. Reproduced from ref. 102 with permission.

ated to a certain extent, were retained the most. In the second direction, the cation-exchange phenomenon was suppressed by the eluent, which consisted of 0.3% ammonia in *m*-cresol. The amino acids were chromatographed in their anionic form. Aspartic acid and glutamic acid, solutes with two negative charges, had the smallest R_F values (Fig. 12). Nineteen proteinic amino acids were resolved.

Still faster amino acid separations on paper were achieved by electrophoresis followed by chromatography with a hydro-organic eluent orthogonally[103,104].

The development of short-fibre cellulose powder for TLC purposes facilitated the chromatography of amino acids and allowed rapid routine analytical work. In all assays reported on cellulose, the mobile phases in both directions were water–organic mixtures[105–111]. Munier *et al.*[109,110] achieved the separation of 22 polar and non-polar amino acids, among which certain pairs that were previously unresolved such as leucine–isoleucine, arginine–lysine and serine–glycine. A high degree of resolution is afforded owing to differences between alcohol–solute interactions in the first direction and ketone–solute and tertiary amine–solute interactions in the second, and to the ionic equilibria created by using 2-methylpyridine together with formic acid in the second eluent. The water content of the mobile phase, by affecting solute partition, plays a determining role in these assays (Fig. 13). Munier *et al.*[110] found a 20% water content in both directions to be optimal. Smaller percentages did not ensure the elution of the most polar amino acids and higher percentages led to decreased resolution.

Kraffczyk *et al.*[107] included a 2 cm wide layer of a strongly acidic ion exchanger at the bottom of the cellulose plate for the desalting of urine samples when analysing

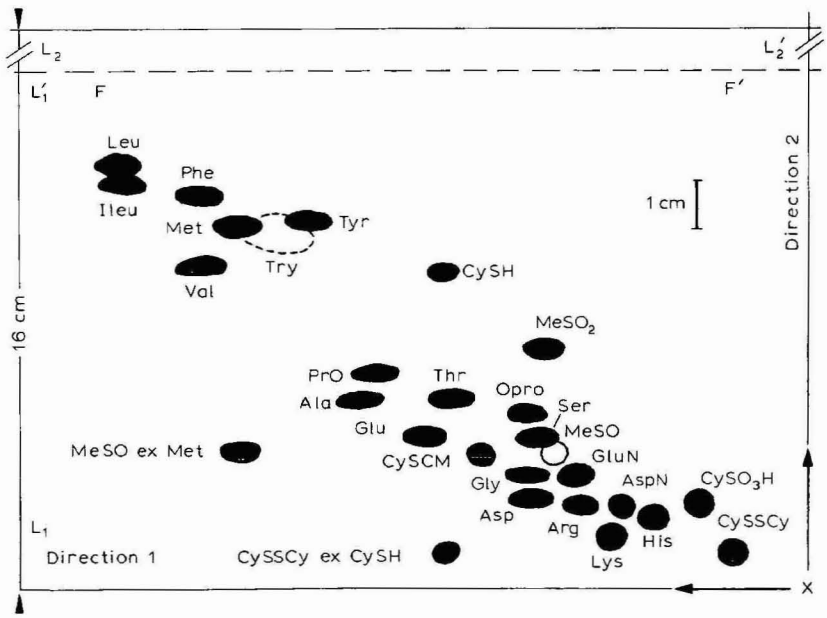


Fig. 13. Two-dimensional separation of amino acids on short-fibre cellulose. Solvent used in the first direction, propanol–formic acid–water (75:5:20), and in the second direction, methyl ethyl ketone–2-methylpyridine–formic acid–water (31:47:2:20). Reproduced from ref. 110 with permission.

TABLE 9

SEPARATION OF Dns- AND DNP-AMINO ACIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
18	Dns-amino acids	Polyamide sheet, 15 × 15 cm		Water–90% formic acid (200:3)			Benzene–acetic acid (9:1)		117
22	Dns-amino acids (renal tubular fluid sample)	Polyamide TLC, Schleicher & Schüll, 3 × 3 cm		4% Formic acid			(a) Benzene–glacial acetic acid (8:2) (b) Ethyl acetate–methanol–glacial acetic acid (20:1:1)		118 (Fig. 14)
39	Dns-amino acids + others (serum and urine samples)	Micropolyamide plates, F1700, Schleicher + Schüll, 4.2 × 4.2 cm	0.5	Formic acid–water (1.5:98.5)	5 min	Dry, hot air, cool to room temp.	Benzene–acetic acid (4.5:1)	5 min	119
19	Dns-amino acids	Kieselgel G, 0.25 mm		Ethyl acetate–chloroform–ethanol–acetic acid (70:45:4:4)			Chloroform–acetic acid–water (50:45:5)		120
19	Dns-amino acids	HPTLC Fertigplatten RP-8 F 254, 10 × 10 cm		*n*-Heptane–ethyl acetate–acetic acid (65:33:2)	7 cm		Methanol–0.01 *M* Na_2HPO_4 (75:25)	7 cm	121
20	DNP-amino acids	RP-18		Hexane–ethyl acetate–acetic acid (80:18:2)	6 cm		1 *M* ammonia + 3% KCl in 60% methanol	6 cm	34 (Fig. 2)
17	DNP-amino acids	Polyamide, 15 × 15 cm, 100°C, 15 min	2.0	*n*-Butanol–glacial acetic acid (90:10)	10 cm, 200 min	Dry, hot air, 15 min	90% formic acid–water (50:50)	11 cm, 60 min	122
18 + 23	DNP- + Dns-amino acids	Cellulose powder, Macherey, Nagel & Co., 30 × 20 cm, 0.11 mm		Toluene–ethylene glycol chlorhydrin–pyridine–0.8 *M* ammonia (150:90:45:90) + a few drops of *n*-octanol	30 cm		Water–water satd. with ammonium sulphate–sodium dodecyl sulphate (700 ml:100 ml:567 mg)	20 cm	124

for urinary amino acids. Other separations on silica gel were reported[112,113]. An organic–basic eluent was used in the first direction followed by an organic–acidic mixture in the second. Solute retention depended on the types of functional groups and their degree of ionization. Ionophoresis followed by chromatography on silica gel has also been applied to the separation of amino acids[114].

4.4.2. Dimethylaminonaphthalenesulphonyl (Dns) and dinitrophenyl (DNP) amino acids (Table 9)

Seiler[116] has reviewed the separations of various Dns-derivatives, among which Dns-amino acids. Two-directional TLC has been achieved on a polyamide stationary phase[117–119] (Fig. 14) and has recently been applied to the identification of human acidopathies in serum and urine[119]. Although Dns-amino acids have also been analysed on silica[120], assays on polyamide are preferred as they are less time consuming, do not result in spot tailing and do not require previous deionization of urine samples[119]. An aqueous eluent is generally used in the first direction followed by an organic eluent in the second. This change in the nature of the mobile phase causes alterations in the sorbent properties such that the mechanisms for solute retention are different in each direction. Polyamide is thought to act as a reversed phase in the presence of the aqueous eluent, and it behaves as a hydrophilic sorbent there-

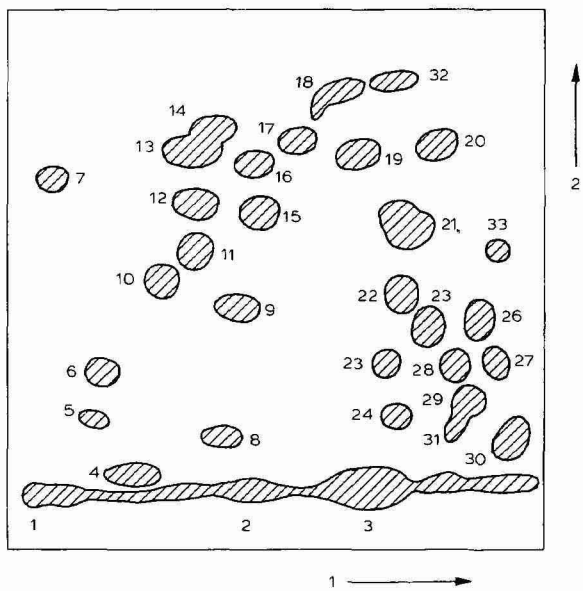


Fig. 14. Two-dimensional chromatogram of some Dns-amino acids on polyamide after autoradiography. 1 = Starting point; 2 = taurine; 3 = Dns-OH; 4 = cystine; 5 = *n*-serotonin; 6 = tryptophan; 7 = bis-tyrosine; 8 = *n*-tyrosine; 9 = ornithine; 10 = bis-lysine; 11 = phenylglycine; 12 = phenylalanine; 13 = leucine and histidine; 14 = isoleucine; 15 = methionine; 16 = norvaline; 17 = valine; 18 = proline; 19 = GABA; 20 = δ-aminolevulinic acid; 21 = alanine and Dns-NH_2; 22 = glycine; 23 = glutamic acid; 24 = aspartic acid; 25 = hydroxyproline; 26 = glutamine; 27 = asparagine; 28 = threonine; 29 = serine; 30 = arginine, ε-lysine and α-lysine; 31–33 = unknown dansylation products. Solvent used in the first direction, 4% formic acid, and in the second direction, benzene–glacial acetic acid (8:2) followed by ethyl acetate–methanol–glacial acetic acid (20:1:1). Reproduced from ref. 118 with permission.

TABLE 10

SEPARATION OF PEPTIDES

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*Solvent 1*	*t/L*	*Solvent 2*	*t/L*	*Ref.*
11	Peptides	Cellulose MN 300, 20 × 20 cm, 0.25 mm	*tert.*-Amyl alcohol–eucalyptol–2-chloroethanol–pyridine–98% formic acid (150:150:200:280:43:200)	Top, 5 h	*n*-Amyl alcohol–pyridine–H_2O (4:4:2)	5 h	125
8	Oligopeptides	Cellulose MN 300, 0.25 mm	Isoamyl alco-hol–ethanol–glacial acetic acid– pyridine–water (17.5:5:1.3:17.5:15) (pH 5.75)		Isopropanol–ethanol–ammonia (20:20:15) (pH 12.3)		126
19	Peptides	Cellulose MN 300, 40 × 20 cm, 0.25 mm	Electrophoresis, 1.04 *N* formic acid, 427 V/40 cm, 8 mA/20 cm × 0.25 mm	3.5 h	*n*-Butanol–pyridine–98% formic acid–water (479:278:43:200)	To top, 3 h	125
19	Peptides	Cellulose MN 30, 40 × 40 cm, 0.25 mm	Pyridine–ethanol–water (4:4:2)	Top, 4 h	Electrophoresis, 0.025 *M* aq. borax soln., 380 V/ 40 cm, 4.5 mA/20 cm × 0.25 mm	4 h	125
	Polypeptides/proteins with acidic or neutral p*I*	(1) Tube gel, polyacrylamide (2) Slab gel, acrylamide gradient	(1) 9 *M* urea, Nonidet P-40, pH 3.5–10 Ampholines, 400–700 V	20 h	(2) Electrophoresis in presence of sodium dodecyl sulphate	3 h	128, 129
	Basic proteins	(1) Tube gel, polyacrylamide (2) Slab gel, acrylamide gradient	(1) Dipalmitoyl-L-α-phosphatidylcholine + urea, pH 3.5–10 Ampholines, 800 V	2.6 h	(2) Unchanged, 3200 V/h		133

after[121]. Thus, whereas the R_F values for arginine and aspartic acid are relatively large in the first direction, they are much smaller in the second[117–119].

Exploiting similar solvent changes with a reversed-phase plate, Macek *et al.*[121] succeeded in resolving 19 Dns-amino acids. The RP-8 TLC plate behaved as a normal phase in presence of the non-aqueous eluent used in the first direction and as a true reversed phase when developed with an aqueous solvent in the second direction. Exact reversal of the retention order of the Dns-glycine, -alanine, -valine and -leucine could be observed in the second direction with respect to the first elution. In addition, the aqueous eluent was basic enough to reduce the amino group ionization and hence to increase solute retention on the reversed-phase plate.

DNP-amino acids were separated under similar conditions on an RP-18 thin-layer plate[34]. It is interesting that the addition of a salt to the non-aqueous solvent did not modify the solute behaviour, whereas it increased the retention when present in the aqueous eluent, a true expression of reversed-phase solvophobic behaviour. Separations of DNP-amino acids were also accomplished on polyamide[122] and cellulose[123,124] by development with an organic solvent in the first direction and an aqueous solvent orthogonally. The efficiency of the chromatographic system required judicious selection of the mobile phase components. Munier and Drapier[124] included a few drops of *n*-octanol in the first eluent in order to suppress the chromatography of the solvent itself. In addition, as impregnation of the plate with the organic mobile phase caused irregularities in the perpendicular progression of the second aqueous solvent, spot tailing and diffusion, sodium dodecyl sulphate was added to this aqueous phase and helped to achieve small and round spots.

4.4.3. Peptides and oligopeptides (Table 10)

Peptides[125] and oligopeptides[126] have been separated on cellulose with an acidic solvent in one direction and a basic solvent in the other. In addition to the differences in solute ionization which originate from the use of eluents at different pH values, differences in molecular weight also affect the retention and the partition process. In a given category of compounds, the dipeptides for instance, solutes with a large number of hydrophobic carbon centres, more soluble in the organic portion of the eluent, exhibit larger R_F values[126].

Other peptide assays on cellulose[125] have combined electrophoresis in one direction and chromatography with an organic–aqueous mobile phase in the other. The electrophoresis step necessitated the use of binder-free cellulose, sufficiently large plates, a weak gradient potential and an adequate electrolyte solution. Peptides migrated according to their charge, the solute pK_a values and the pH of the electrolyte.

4.4.4. Proteins

Although not related to TLC, the high-resolution, two-dimensional electrophoretic method developed by O'Farrel[127] and later by Anderson and co-workers[128–136] should also be mentioned. Nearly 1000 spots were obtained from such an analysis of lymphocyte proteins using autoradiography (Fig. 15). More sensitive detection techniques are expected to afford the resolution of about 5000 components.

In the first dimension, proteins or polypeptides were separated according to their charge by isoelectric focusing in a narrow gel tube. Next, the gel was extruded and positioned on a polyacrylamide gradient slab, and electrophoresis was performed

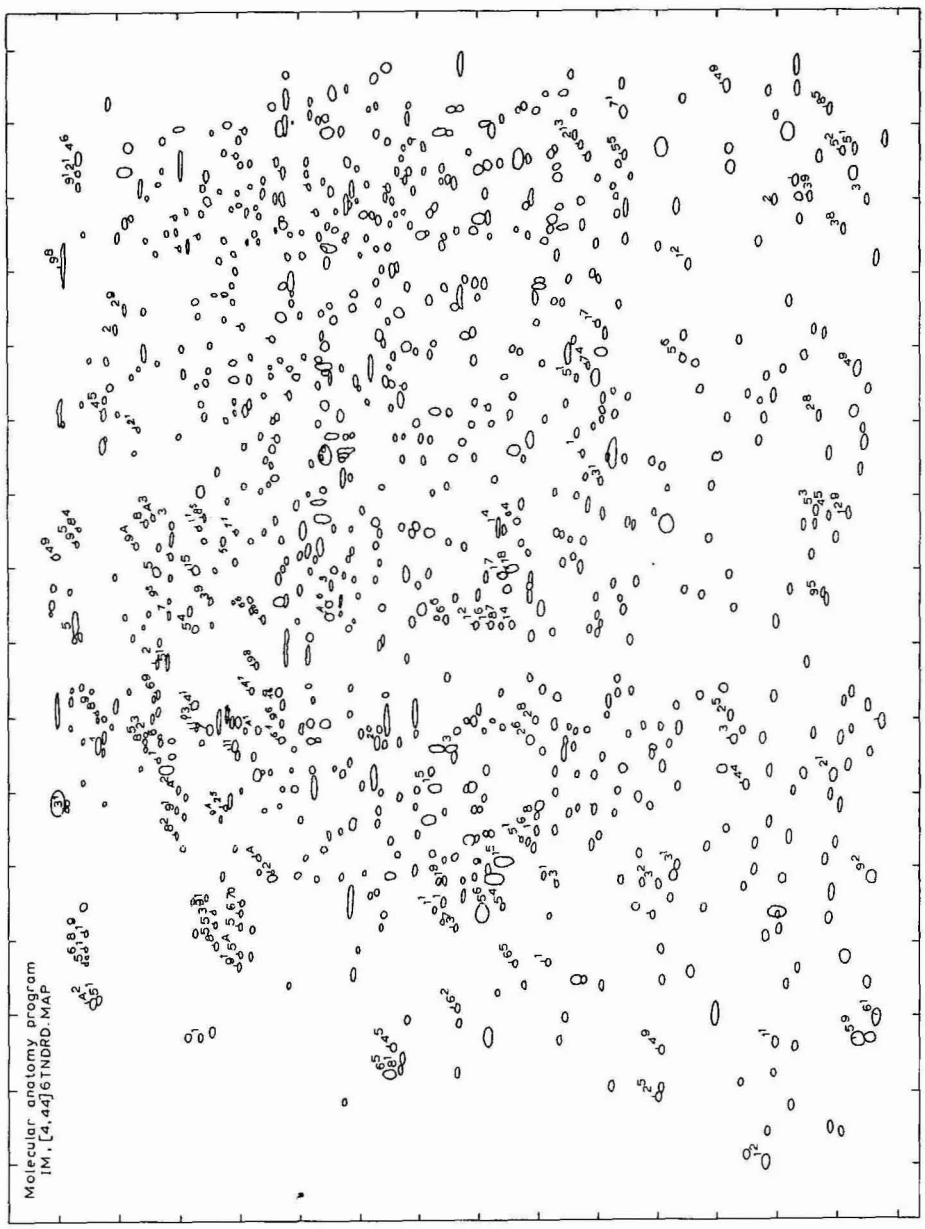


Fig. 15. Diagram showing the spots resulting from the two-dimensional gel electrophoresis of lymphocyte proteins. Numbers are the key to information about the respective spots in the lymphocyte protein index data base developed by Anderson *et al.* For further details see ref. 48. Reproduced from ref. 48 with permission.

in the presence of sodium dodecyl sulphate. In this second dimension, compounds were resolved according to their molecular weight, as sodium dodecyl sulphate binds electrostatically to the solutes, thus masking charge differences (Table 10).

The method described was applied successfully to a study of the protein constituents of physiological fluids and tissues in normal and diseased individual. [49,50,129–131,134,135,137–140]

Because of the considerable number of proteins that can be separated in one analysis, data handling becomes very complex as huge files have to be stored and monitored. The corresponding software has been developed by Anderson *et al.*[48] and Lester *et al.*[49]. A discussion of the problems of spot detection, segmentation, integration and pairing is beyond the scope of this review.

4.5. Carbohydrates (Table 11)

Sugars have been separated on cellulose[141] and Kieselgel G[142], developed with different water–organic solvents. Hotta and Kurokawa[143] modified a silica gel plate by dipping it in 0.2 *M* sodium dihydrogen phosphate solution, a procedure known to enhance sugar retention in proportion to the number of hydroxyl substituents[144]. This selective stationary phase was developed with an eluent containing 10% of water in the first direction and 25% in the second.

The effect of water on chromatographic mechanisms can be illustrated by the behaviour of rhamnose and fucose in each eluent. These sugars differ in the steric arrangement of their functional groups: rhamnose has one pair of *cis*-hydroxyl groups in a β-position with respect to a bulky methyl group, compared with two pairs of *cis*-hydroxyl groups in fucose, one β- and one α- to the methyl group. With the first eluent, the adsorption of rhamnose may be more sterically hindered than that of fucose and thus rhamnose migrates faster. These structural differences are no longer important with the second eluent, as solute adsorption on to silica is reduced owing to plate deactivation by water present in the mobile phase. The solutes then are believed to partition between the mobile and the modified stationary phases, which results in similar R_F values for rhamnose and fucose (Fig. 16).

Carbohydrates have also been separated on silica gel impregnated with sodium tetraborate, sodium tungstate[145] and boric acid[144]. In the first direction, a neutral solvent was used and sugars were retained according to their capacity to form borate complexes. In the second elution, the impregnating agent was completely deactivated by the acidic solvent. Solute partition was in effect and the heavier disaccharides were retained the longest. Phenylboronic and boric acids have more recently been used in the mobile phase to resolve carbohydrates on silica[146]. Other separations have been accomplished on cellulose developed in different mobile phases[147].

4.6. Glycopeptides

Moczar[148] reported the separation of some glycopeptides from a glycoprotein enzymatic digest on silica. Electrophoresis in presence of acetic acid–pyridine–water (10:1:89) (pH 3.8) was performed for 2–3 h at 10–20 V/cm on a 20 × 20 cm plate. This operation was followed by a continuous development with ethanol–nitromethane–acetic acid–water (5:3:3:3) for 18–30 h.

TABLE 11

SEPARATION OF CARBOHYDRATES

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
12	Sugars	Cellulose MN 300 G, 110°C, 10 min	2	*n*-Butanol–acetone–diethylamine–water (10:10:2:5)		80°C, 30 min	Vapour phase equilibrated with 25% ammonia, phenol–water (3:1)		141
4	Man, Gal, Glc-NAc, Man, 1-6-Man, Gal-β1-4-Glc-NAc	Kieselgel G (Merck)		*n*-Butanol–acetic acid–water (12:3:5)	16 h		*n*-Propanol–ethyl acetate–water (7:2:1)	6–8 h	142
8	NANA, Gal, Glc, Man, Gal-NAc, Glc-NAc, Fuc, Rham	Si gel F_{254} dipped in 0.2 *M*′sodium dihydrogen phosphate, 110–120°C, 30 min, 20 × 20 cm, 0.25 mm		Butanol–acetone–water (4:5:1) (2 ×)	15 cm		Phenol–water (3:1) (2 ×)		143 (Fig. 16)
40	CHO, including deoxy sugars and methylglycosides	Si gel: (1) 4.2 cm, impregnated with sodium tetraborate–boric acid–sodium tungstate (2) 14.5 cm, impregnated with boric acid		On (1): methyl acetate–isopropanol–water (2:2:1)		550°C <3 h	On (2): ethyl acetate–acetic acid–methanol–water (60:15:15:10)		144
16	CHO,	Sodium tetraborate–sodium tungstate impregnated silica, 20 × 20 cm, 0.3 mm, 90°C, 30 min		Ethyl acetate–isopropanol–water (2:2:1)	2 h	70°C, 4–5 h	Ethyl acetate–acetic acid–methanol–water (60:15:15:10)	50 min	145
13	Sugars	Si gel 60 (Merck)		(a) Ethyl methyl ketone–diisopropyl ether–2-propanol–pyridine–water–phenylboronic acid (40:10:30:10:10:1.2)	10 cm		(b) Diisopropyl ether–methanol–acetic acid–water (88:12:2:2) (c) Ethyl methyl ketone–2-propanol–acetonitrile–0.5 *M* boric acid + 0.25 *M* isopropylamine–acetic acid (40:30:20:15:0.4)	10 cm	146
15	Sugars	Cellulose, 20 × 20 cm, 0.1 mm		2-Propanol–90% formic acid–water (80:4:20)	5–6 h		Lutidine (2,6-dimethylpyridine)–water (65:35)	6 h	147

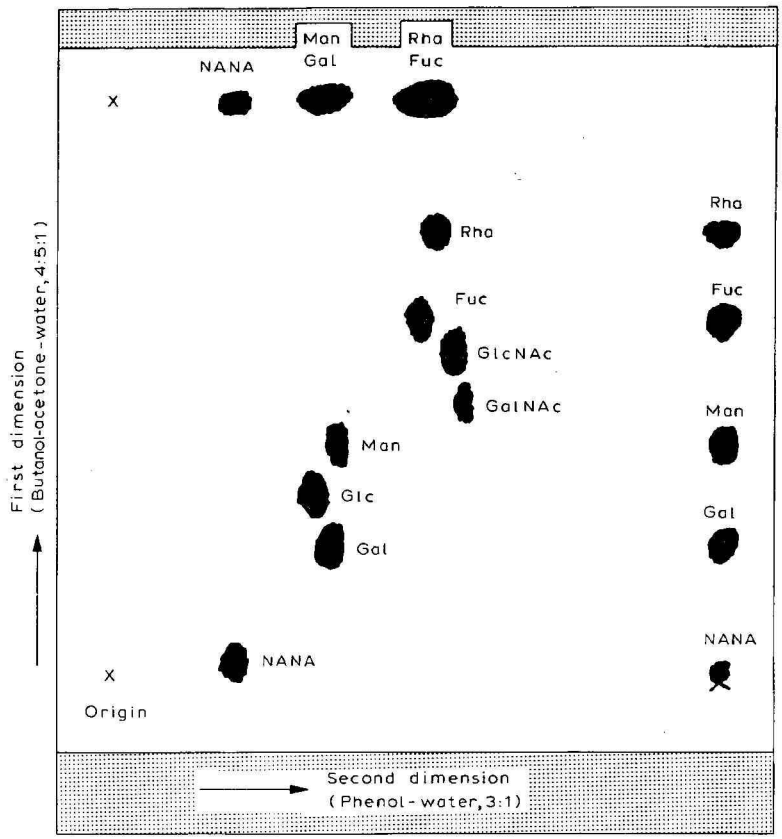


Fig. 16. Two-dimensional TLC of sugar mixture on silica gel dipped in 0.2 *M* sodium dihydrogen phosphate. Rha = rhamnose; Fuc = fucose; GlcNAc = acetylglucosamine; GalNAc = acetylgalactosamine; Man = mannose; Glc = glucose; Gal = galactose; NANA = N-acetylneuraminic acid. First direction: two successive developments in butanol–acetone–water (4:5:1). Second direction: two successive developments in phenol–water (3:1). Reproduced from ref. 143 with permission.

More recently, the soluble inhibitory factor (SIF), a molecule constituted of both protein and glycolipid moieties, has been isolated from serum and purified on a silica plate using chloroform–methanol–water in the proportions 60:38:8 in the first dimension and 50:50:5 in the second[149].

4.7. Nucleic acids and their constituents

In cells, nucleic acids are carriers of genetic information and their constituents, the free bases, nucleosides and nucleotides, actively participate in cellular metabolism. Detailed conditions for the two-dimensional separation of these compounds are given in Tables 12 and 13.

4.7.1. Bases, nucleosides and nucleotides (Table 12)

Randerath and Randerath[150] achieved the first rapid, bi-directional separation of 23 ribonucleotides on PEI-cellulose. Several mono-, di- and trinucleotides were

TABLE 12

SEPARATION OF NUCLEOTIDES, NUCLEOSIDES AND BASES

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
23	Ribonucleotides	PEI, cellulose, 20 × 20 cm, 0.5 mm		(a) 0.2 *M* LiCl (b) 1.0 *M* LiCl (c) 1.6 *M* LiCl	2 min 6 min 13 cm or 75 min	Air, < 50°C, wash LiCl in CH_3OH	(d) 0.5 *M* formate buffer (pH 3.4) (e) 2.0 *M* formate buffer (f) 4.0 *M* formate buffer	30 sec 2 min 15 cm or 60 min	150 (Fig. 17)
8	2′-, 3′-G, A, U, CMP	PEI, cellulose MN 300	3	1.0 or 0.1 *N* formic acid (pH 3.6)	10–15 cm	Air	1 *M* LiCl (pH 7.0)	8 cm	151
9	Adenine + pyridine phosphates	PEI, cellulose (Brinkmann) 20 × 20 cm, 0.1 mm	3	0.5 *M* formate buffer (pH 3.6)		Dry, wash in CH_3OH, dry	0.2 + 1.0 *M* LiCl		152
14	Phosphate esters	Cellulose MN 300, 20 × 17.5 cm, 0.25 mm		*n*-Propanol–ammonia–water (6:3:1) (2 ×)	3 h		*n*-Propyl acetate-90% formic acid–water (11:5:3) (2 ×) or electrophoresis with 0.28 *M* acetate buffer (pH 3.6), 1000 V, 35 mA	80 min 16 min	153
22	Nucleosides, nucleotides	Cellulose MN 300		Isobutyric acid–conc. ammonia–water (57:4:39)			Methanol–1 *M* ammonium acetate (7:3) (2 ×)		154
8	2′-, 3′-G, A, U, CMP	Cellulose MN 300, 100°C, 30 min, 20 × 20 cm, 0.5 mm	3	*n*-Butyric acid–ammonia–water (57:4:39)	5–6 h, 12–15 cm	Overnight in hood	Sat. ammonium sulphate–1 *M* sodium acetate–isopropanol (79:19:2)	3–4 h, top	155

8	5′-O-Methyl-Nucleotides	Cellulose		Isobutyric acid–0.5 *N* ammonia (5:3)			Isopropanol–conc. HCl–water (17:15:15)		156
5	Bases: A, C, G, T, bromo-U	Cellulose (Eastman 6065), 3.5 × 20 cm, 20 × 20 cm (2 layers)	2	Isopropanol–water–HCl (65:18.4:16.6)	14 cm 6 h		1 *M* disodium hydrogen phosphate–1.2 *M* ammonium sulphate–isopropanol (123:74:3)	12 cm 1 h	36
37	Purine and pyrimidine nucleosides and bases (not all resolved) in urine	Cellulose DC-Alufolien, 10 × 10 cm, 0.1 mm	1.5	Isopropanol–5% ammonia (8:2) (2 ×)	90 min		Butanol–acetic acid–H_2O (8:2:2) (2 ×)		157
44	Bases, nucleosides, nucleotides (not all resolved)	Cellulose MN 300, 20 × 20 cm, 0.5 mm	3	*n*-Propanol–25% ammonia–water (6:3:1)	3 h, 18 cm	Cold air, 20 min	Isopropanol–sat. ammonium sulphate–water (2:79:19)	3 h	158 (Fig. 18)
19	Bases, nucleosides, nucleotides	Polygram CEL 400, UV 254 nm, 10 × 10 cm		(a) Methanol (b) Methanol–isopropanol–25% (w/w) ammonia–1% (w/v) EDTA (3:9:2:6) (c) Solvent (b)	Middle Top		(d) Isobutyric acid–25% (w/w) ammonia–1% (w/v) EDTA (200:9:114)	Top	159
22	Methylated tRNA bases	Si–cellulose (40:60), 20 × 20 cm, 0.4 mm, desiccated	2–3	Ethyl acetate methanol–water–88% formic acid (100:25:20:1)	150 min	60 min	Acetonitrile–ethyl acetate–2-propanol–1-butanol–58% ammonia–water (40:30:20:10:22:5)	150 min	162
13	Bases, nucleosides, nucleotides	Si gel (Merck) HPTLC F_{254}, 10 × 10 cm	2	1-Butanol–acetone–acetic acid–5% ammonia–water (10:5:2:3:2)	7 cm	Thorough drying	1-Propanol methanol–ammonia water (10:1:5:2)		163

resolved, as well as some nucleotide sugars. Increasing concentrations of lithium chloride solutions and formate buffer (pH 3.4) were used stepwise in the first and second directions, respectively. Compared with elution at constant concentration, step-gradient elution resulted in sharper circular spots. Solutes were resolved according to their charge: the most negatively charged trinucleotide species migrated the least on the PEI anion exchanger (Fig. 17). Similar conditions were later applied by Santini and Ulrich[151] to the separation of 2'- and 3'-adenine, guanine, uridine and cytosine monophosphates, and by Barton *et al.*[152] to that of nine pyridine and adenine nucleotides.

Various phosphate esters[153,154], 2'- and 3'-monophosphates[155], 2',O-methyl nucleotides[156], purine and pyrimidine bases[36] and nucleosides[157] have also been chromatographed on cellulose. The pH of the eluent, which affects the extent of solute dissociation, plays an important role in these assays. Thus, in most instances, development was accomplished with an acidic solvent in one direction and a basic solvent in the other.

The use of a basic solvent has been coupled with that of a salt in order specifically to affect nucleotide retention[158,159]. A mixture of 44 bases, nucleosides, deoxynucleosides, 2'-, 3'- and 5'-nucleoside monophosphates, nucleoside di- and triphosphates and nucleotide sugars was resolved by Pataki[158] on cellulose. The eluents were *n*-propanol–25% ammonia–water (5:3:1) in the first direction and isopropanol–saturated ammonium sulphate–water (2:79:19) in the second. Triphosphates were retained the most with the first eluent. The second buffer system enhanced their migration whereas it hardly affected the position of nucleosides and bases (Fig. 18). Randerath and Randerath[160] had previously observed these ionic strength effects on the chromatographic behaviour of nucleic acid constituents.

Using a silica gel–cellulose plate with acidic and basic solvents, Munns and co-workers[161,162] resolved 22 methylated tRNA purine and pyrimidine bases. Solutes with primary amine groups such as adenine, guanine and cytosine exhibited lower R_F values in a formic acid than in an ammonia system. These differences were found to arise from interactions with silica, the adsorption of the primary amines also being decreased by their methylation. At a basic pH, both the bases and the silica phase are negatively charged, which weakens adsorbent–solute interactions.

Finally, Das[163] separated 13 bases, nucleosides and nucleotides on pure silica by varying the solvent pH and composition in the second direction.

4.7.2. Oligonucleotides and nucleic acids (Table 13)

Miller and Burgess[164] resolved five oligonucleotides on PEI-cellulose by means of lithium chloride–EDTA solution at pH 6.5 in the first direction and at pH 2.0 in the other. The charges on both the phosphate and base moieties affected the separation. Also by varying the pH of the eluent, Mirzabekov and Griffin[165] were able to separate 18 oligonucleotides on PEI-cellulose. The first direction involved successive developments with 1.4 and 1.8 *M* solutions of lithium formate at pH 3.4; the lower concentration ensured the resolution of smaller oligonucleotides and the higher one that of the larger solutes. The second eluent was 0.8 *M* lithium chloride solution in Tris base at pH 8.0. The chromatographic assay was carried out at 60°C for sharper spot formation. Migration in the first direction was according to charge and nucleotide composition whereas in the second direction it was more a function of molecular

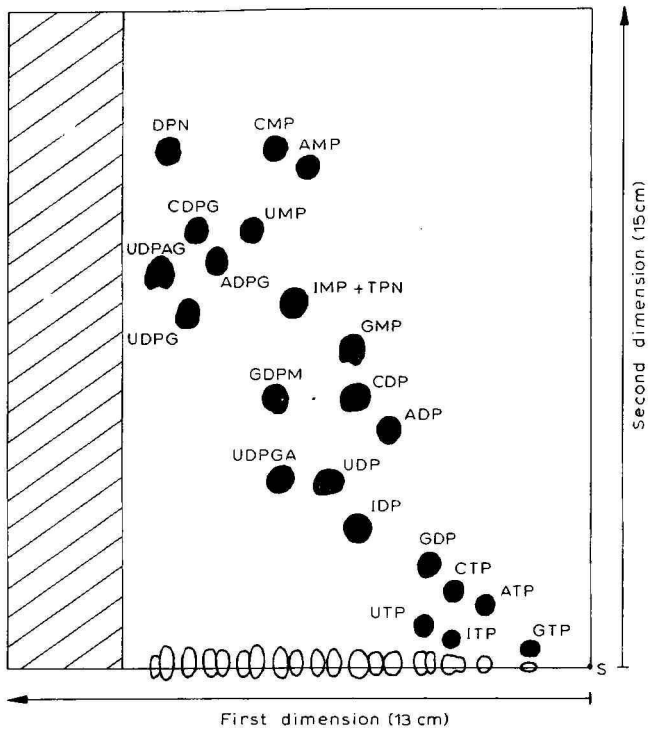


Fig. 17. Two-dimensional anion-exchange separation of nucleotides on PEI-cellulose. First dimension: successive developments in (a) 0.2 *M* LiCl, (b) 1.0 *M* LiCl, (c) 1.6 *M* LiCl. Second dimension: successive developments in (d) 0.5 *M* formate buffer (pH 3.4), (e) 2.0 *M* formate buffer, (f) 4.0 *M* formate buffer. CMP = cytosine 5′-monophosphate; AMP = adenosine 5′-monophosphate; CDPG = cytidine diphosphate glucose; UMP = uridine 5′-monophosphate; UDPAG = uridine diphosphate-N-acetyl-glucosamine; ADPG = adenosine diphosphate glucose; IMP = inosine 5′-monophosphate; GMP = guanosine 5′-monophosphate; GDPM = guanosine diphosphate mannose; CDP = cytosine 5′-diphosphate; ADP = adenosine 5′-diphosphate; UDPGA = uridine diphosphate glucuronic acid; UDP = uridine 5′-diphosphate; IDP = inosine 5′-diphosphate; GDP = guanosine 5′-diphosphate; CTP = cytosine 5′-triphosphate; ATP = adenosine 5′-triphosphate; UTP = uridine 5′-triphosphate; ITP = inosine 5′-triphosphate; GTP = guanosine 5′-triphosphate; DPN = nicotinamide adenine dinucleotide; TPN = nicotinamide adenine dinucleotide phosphate. Reproduced from ref. 150 with permission.

weight. More complex mixtures of half or whole 5S-RNA molecules were resolved by continuous gradient elution. The concentrations of the salt in the eluents depended on the fragments to be separated, the chromatography of a whole 5S-RNA molecule requiring 4.5 *M* lithium formate.

The separation of more than seven methylated mRNA 5′-termini, achieved by Gross *et al.*[166] on cellulose, again involved different ionic equilibria in each direction and their effect on solute migration patterns. Faster assays on cellulose have been reported by Bergquist[167], who separated 17 oligo- and mononucleotides by coupling electrophoresis with TLC. The system described is extremely powerful, capable of resolving tetra- or oligonucleotides of similar charge and chain length.

The combination of gel electrophoresis and TLC has more recently been applied to RNA sequencing studies[168]. First, 3′-terminal RNA half-molecules are sep-

TABLE 13

SEPARATION OF OLIGONUCLEOTIDES AND NUCLEIC ACIDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (in.)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
5	5′-RNA terminal oligonucleotides	PEI, cellulose MN 300, Brinkmann, 20 × 20 cm	1	2.0 *M* LiCl + 0.01 *M* EDTA (pH 6.5)	Top	Wash in CH_3OH, dry	3 *M* LiCl + 0.01 *M* EDTA–3.6 *M* formic acid (pH 2.0, adjusted with solid LiOH)		164
18	Oligonucleotides (T1 RNase digest of 5S RNA)	PEI, cellulose MN 300, 20 × 20 cm		(a) 1.4 *M* lithium formate in 7 *M* urea (pH 3.4), 60°C (b) Above mixture, 1.8 *M* (pH 3.4), 60°C	10 cm, top	Wash in CH_3OH, dry	(c) 0.8 *M* LiCl in 0.02 *M* TMS base and 7 *M* urea (pH 8)		165
	Partial fragments of 5S RNA	PEI, cellulose MN 300, 20 × 20 cm		4.0 *M* lithium formate in 7 *M* urea; gradually introduce 7.5 *M* above solution (pH 3.4)			1.0 *M* LiCl in 7 *M* urea; gradually introduce 3.2 *M* LiCl (pH 8), 60°C		165
>7	Methylated mRNA 5′-termini	Cellulose (Merck), 20 × 20 cm		Isobutyric acid–ammonia–water (pH 23.7) (66:1:33)	8 h	Hood, overnight	Sat. ammonium sulphide–1 *M* sodium acetate (pH 5.5)–propan-2-ol (40:9:1)	6-7 h	166
17	Oligonucleotides + mononucleotides	Cellulose MN 300, 20 × 20 cm, 0.25 mm		Electrophoresis with 0.1 *M* ammonium formate (pH 2.45) containing 0.001 *M* EDTA, 50V/cm, 16–20 mA	20-25 min	Dry under IR lamp	*tert.*-Butanol–0.08 *M* formic acid–isoamyl alcohol (50:50:2)	10 cm, 4 h	167
	(1) Oligonucleotides (2) Nucleotide sequencing	(1) Gel electrophoresis (2) DEAE-cellulose		(1) Electrophoresis			(2) 15 m*M* sodium citrate buffer (pH 3.1)		168
17	Oligonucleotides	(1) Cellulose acetate paper strips (2) DEAE-cellulose plates		(1) Electrophoresis (pH 3.5)			(2) Homochromatography		169

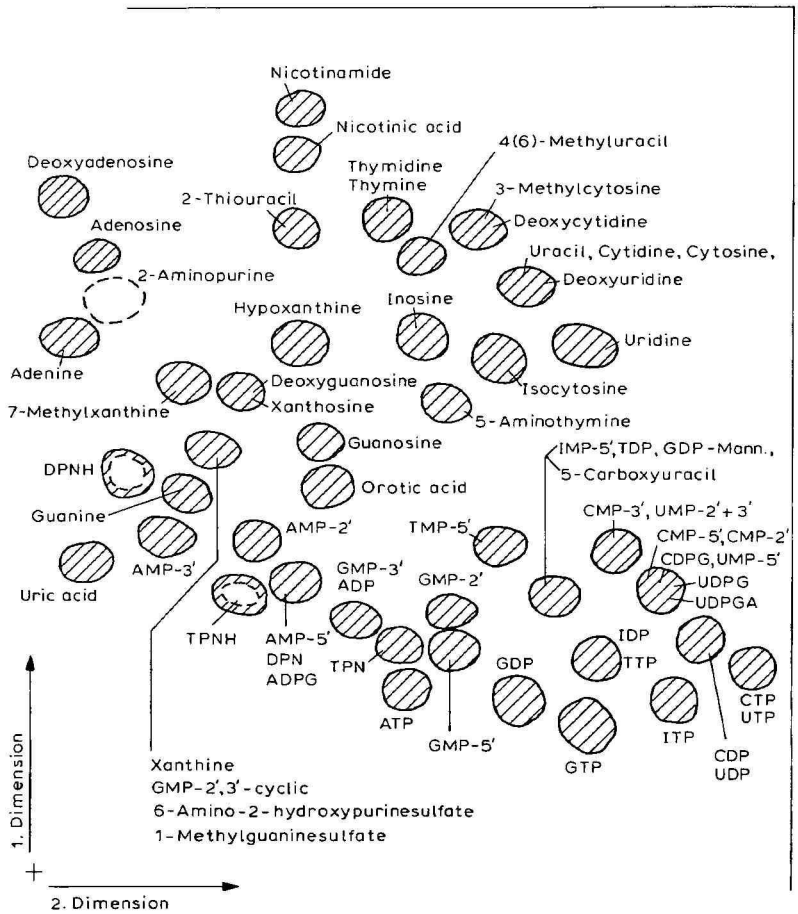


Fig. 18. Two-dimensional separation of nucleo-derivatives on purified cellulose layers. First dimension, *n*-propanol–25% ammonia–water (6:3:1); second dimension, isopropanol–saturated ammonium sulphate–water (2:79:19). Absorption spots are hatched, fluorescence spots are surrounded by broken lines. Reproduced from ref. 158 with permission.

arated by gel electrophoresis. Then, the entire ladder of bands is excised from the gel, transferred to a thin layer of DEAE-cellulose by blotting and hydrolysed *in situ* with takadiastase RNAase. The thin layer is developed in a direction perpendicular to gel electrophoresis with 15 m*M* sodium citrate buffer (pH 3.1). The enzyme is supposed to hydrolyse one nucleotide at a time and thus the resulting pNp spots correspond to the sequence of nucleotides in the original RNA molecule.

4.8. Environmental pollutants (Table 14)

It is of interest for the environmental chemist to identify and quantify polyaromatic hydrocarbons and aza heterocycles in air samples from different sources. This was achieved by Sawicki and co-workers[170–176], who analysed by two-dimensional TLC extracts obtained directly or after column fractionation of airborne particulate and coal-tar pitch fume samples.

TABLE 14

SEPARATION OF ENVIRONMENTAL POLLUTANTS: AZAARENES AND POLYNUCLEAR AROMATIC HYDROCARBONS (PAHs)

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
8	Azaarenes + others	Al_2O_3		Cyclohexane–ethyl acetate (1:1)	15 cm		Toluene	15 cm	170
33	Benzene-soluble fraction of airborne particulate sample; acridine, pyrene, benz[*c*]acridine identified	Alumina–cellulose (2:1), 20 × 20 cm, 0.25 mm		Pentane	15 cm		DMF–water (35:65)	15 cm?	173
41	Benzene-soluble airborne particulate fraction with anthracene + other PAHs	Alumina–cellulose acetate (2:1)		Pentane	15 cm		Ethanol–toluene–water (17:4:4)	15 cm	173
65	Coal-tar pitch basic fraction with various azaarenes	Si gel–cellulose (2:1), 20 × 20 cm	1.5 cm from base	Pentane–diethyl ether (9:1)	13 cm, 3 h		DMF–water (35:65)	13 cm, 4.5 h	177 (Fig. 19)
67 or 15	Tokyo air with various PAHs; PAH reference solutions	(1) Alumina, 4 × 20 cm (2) 26% acetylated cellulose, 16 × 20 cm, 0.3 mm. 1 h, 110°C, store at 20% humidity		On (1): *n*-hexane–diethyl ether (19:1) with sat. potassium acetate, 2% humidity	15 cm, 35 min	Air, 5 min	Methanol–diethyl ether–water (4:4:1) (3× for Tokyo air sample)	10 cm, 55 min	178
Numerous	Benzene-enriched airparticulate extract; no spot identification	Chemically bonded phase, 5 × 5 cm		Methanol–water (97:3)	2 min		Methanol–acetonitrile	4 min	184

Of all of the compounds in an airborne particulate, benzene-soluble, "oxy" fraction, compounds with an aza nitrogen such as 9-acridone and 6(5H)-phenanthridone exhibited the longest retention on an alumina plate. Substitution of the aza nitrogen by an oxygen atom or sulphur weakened adsorption, xanthen-9-one and thioxanthen-9-one migrating faster than 9-acridone[170].

In their assay on an alumina–cellulose (2:1) mixed sorbent plate, Sawicki *et al.*[173] used an organic eluent for the first elution. Compounds were primarily retained by adsorption; acridine had the smallest and pyrene the largest R_F values. In the orthogonal direction, the plate was developed with a solvent containing 65% of water. Water interfered with solute adsorption on alumina and also impregnated the cellulose fibres, creating a partitioning medium. Under these conditions, acridine migrated further than pyrene.

Similar mechanisms were effective in the two-dimensional separation of coal-tar pitch aza heterocyclic on a silica–cellulose (2:1) plate. Adsorption on to silica prevailed on development with the organic eluent: owing to the steric hindrance of its aza nitrogen, benzo(*h*)quinoline was less retained than benzo(*f*)quinoline (Fig. 19). In the orthogonal direction, compounds were separated according to their partition coefficients: the bulky dibenz(*a,j*)acridine was retained the most whereas acridine, benzo(*h*)- and benzo(*f*)quinoline had the largest R_F values; in general, retention increased with the number of additional aromatic substituents[177].

Matsushita and Suzuki[178] succeeded in resolving the polyaromatic hydrocarbons anthracene, phenanthrene, pyrene, benz(*c*)anthracene, chrysene, perylene, coronene, benz(*a*)- and benz(*c*)pyrene, benzophenylene, dibenzanthracene and dibenzopyrene. The first development was carried out on an alumina strip with an organic eluent. Adsorption increased with aromaticity and was affected by steric factors. The second development was performed on the acetylated cellulose part of the plate with a polar eluent. Compounds were separated by partition, those with the smallest number of rings migrating further than the others.

Polyaromatic hydrocarbons have more recently been separated on acetylated cellulose[179] and on an acetylated cellulose–silica gel–alumina sorbent mixture[180]. Other methods had involved the use of GC and TLC in combination[181,182]. Janák[182] and Kaiser[183] reviewed in depth both the instrumentation and the applications of this technique.

4.9. Pesticides

Various pesticides, including aldrin and dieldrin[185], DDE and DDT analogues[186], organophosphorus[187] and other compounds[188–190], have been separated on silica plates developed with different solvents in two directions (Table 15).

From the chromatographic behaviour of Planavin and its substituted 4-methylsulphonylaniline derivatives, it could be seen that the propylation of a primary amine weakens its adsorption on to silica, whereas its substitution by a hydroxyl group increases the retention[188]. The chlorination of phenol or benzoquinone also decreases their retention on a silica plate[190].

Yasuda's[189] separation of various substituted benzenes, phenols and anilines on a silica gel–zinc dust plate show that retention generally decreases in the order phenol > aniline > N-methylaniline > benzene > chlorobenzene (Fig. 20). In the

TABLE 15

SEPARATION OF PESTICIDES

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (cm)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
3	Dieldrin, *p,p'*-TDE, aldrin from interferences	Alumina, 10 × 20 cm	3	*n*-Heptane	10 cm	Air, 15 min	Acetonitrile saturated with *n*-heptane		185
10	*p,p'*-DDE + DDT analogues from PCBs	Kieselgel G-HR HN + $AgNO_3$ (chromogenic agent), 20 × 20 cm, 0.25 mm, 80°C, 20 min	3	*n*-Heptane	10 cm, 15–20 min	Air, 5–10 min	*n*-Heptane-acetone (98:2)	10 cm	186
16	Group I organophosphorus pesticides	Si gel G, 20 × 20 cm, 0.25 mm, no activation if <60% humidity; if >60%, 110°C, 1 h	3.8 cm, bottom	Toluene	10 min	30 sec exposure to bromine vapours, chromatography of oxidation products in other directions	25% heptane in ethyl acetate	5 min	187
10	Group II organophosphorus pesticides	idem		25% Heptane in ethyl acetate	10 min	idem	Ethyl acetate	5 min	187
12	Planavin herbicide + related compounds	Si gel F_{254} (Merck), 20 × 20 cm, 0.25 mm		Hexane–ethyl acetate–THF (66:30:4) (2×)			Benzene-acetonitrile (3:2)		188
23	Tetryl and related compounds	Si gel G–Zn (30:0.5, w/w), 110°C, 2 h		Chloroform	55 min	Air, 10 min	Ethyl acetate–light petroleum (1:3)	55 min	189 (Fig. 20)
9	Chloranil + chlorinated derivatives of *p*-benzoquinone, hydroquinone + phenol	Reflex Si gel foils (Kavalier), UV 254 nm, 12 × 12 cm, 0.3 mm, 120°C, 60 min	1.5	Chloroform–benzene (1:6.78)	10 cm		*n*-Heptane-carbon tetrachloride (1:11.56)	10 cm	190

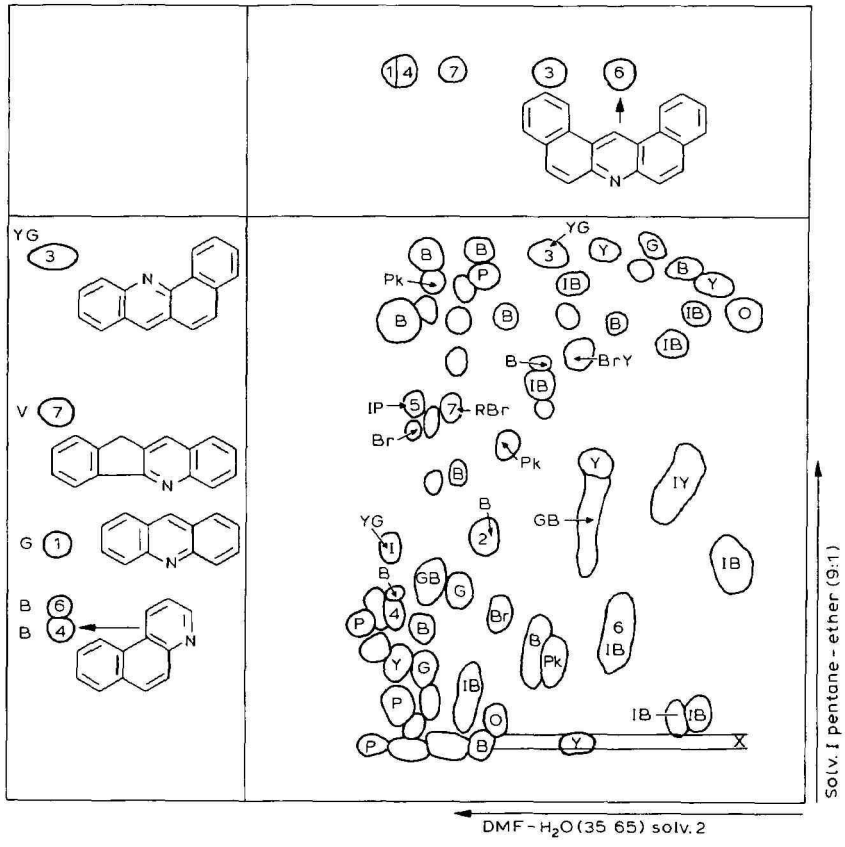


Fig. 19. Two-dimensional thin-layer chromatographic separation on silica gel–cellulose (2:1) of basic fraction equivalent to 2 mg of coal-tar pitch and the characterization of seven spots. Standards: (1) acridine; (2) benz[*a*]acridine; (3) benz[*c*]acridine; (4) benzo[*f*]quinoline; (5) benzo[*h*]quinoline; (6) dibenz[*a,j*]acridine; (7) 11H-indeno[1,2-*b*]quinoline. The plate was sprayed with trifluoroacetic acid fumes and the fluorescence colours were marked. B = blue; Br = brown; G = green; l = light; P = purple; Pk = pink; R = red; Y = yellow; O = orange; V = violet; – = no fluorescence; so located by the quenching of the fluorescent plate. Reproduced from ref 177 with permission.

second direction, differentiation was further made between *meta*-, *ortho*- and *para*-isomers. The elution order may appear surprising at first, as *m*-nitroaniline, a 35-fold stronger base than *p*-nitroaniline, is less retained on the acidic silica phase. Similarly, 3,5-dinitroaniline is less retained than 2,4-dinitroaniline. This may be attributed to the effect of zinc dust in the sorbent mixture.

Gardner's[187] assay of organophosphorus pesticides is one of the few that uses solute derivatization prior to the second plate development. This was accomplished in order to obtain, in the second direction, a widely different migration pattern from the first. The resulting spots are then more separated, which allows better identification of multiple pesticide residues. Thus, after the first development, the plate was exposed to bromine vapour, which converted the thionate and dithioate pesticides into their corresponding oxygen analogues. The plate was then chromatographed with a more polar solvent in a direction perpendicular to the first one.

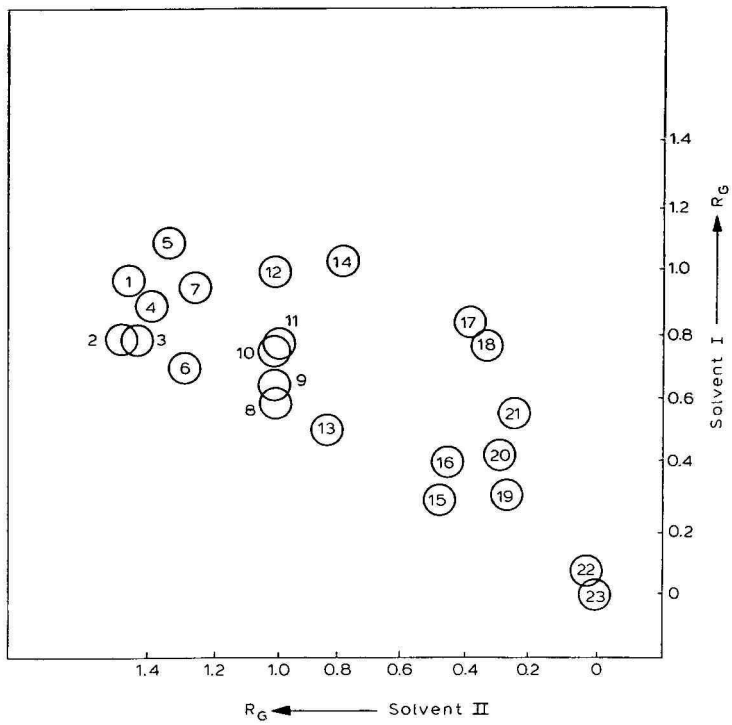


Fig. 20. Two-dimensional separation of tetryl and related compounds on a silica gel G–zinc plate (30:0.5, w/w). 1 = 1-Chloro-2,4,6-trinitrobenzene (picryl chloride); 2 = N,N-dimethylaniline; 3 = 1,3,5-trinitrobenzene (TNB); 4 = 2,4,6-trinitroanisole; 5 = 1-chloro-2,4-dinitrobenzene; 6 = N-methylaniline; 7 = N-methyl-2,6-dinitroaniline; 8 = 2,4,6-trinitroaniline (picramide); 9 = N,2,4,6-tetranitroaniline; 10 = N-methyl-2,4,6-trinitroaniline; 11 = *o*-nitroaniline; 12 = 1,3-dinitrobenzene (reference compound); 13 = N-methyl-N,2,4,6-tetranitroaniline (tetryl); 14 = 1-chloro-2,6-dinitrobenzene; 15 = 3,5-dinitroaniline; 16 = *m*-nitroaniline; 17 = 2,4-dinitroanisole; 18 = N-methyl-2,4-dinitroaniline; 19 = 2,4-dinitroaniline; 20 = *p*-nitroaniline; 21 = N-methyl-N,2,4-trinitroaniline; 22 = 2,4-dinitrophenol; 23 = 2,4,6-trinitrophenol (picric acid). Solvent I, chloroform; solvent II, ethyl acetate–light petroleum (1:3). Reproduced from ref. 189 with permission.

4.10. Inorganic compounds

Perhaps the most important application of the two-dimensional separation of inorganic compounds is shown in Fig. 21, where polyphosphates are separated according to both their type and their chain length. This is achieved by combining an alkaline and an acidic solvent[191].

In the separation of metal ions, two possibilities have been explored, as follows.

(1) The separation is effected using different kinds of complex formation in two directions. This is only feasible, however, if complexant I is volatile or does not interfere with complexant II. A typical example of the latter is shown in Fig. 22. The first solvent (methanol–ethanol–2 *N* hydrochloric acid) separates metal ions mainly according to hydration differences and complexation with hydrochloric acid at low acid concentrations. The second solvent separates according to the extraction of complexes at high hydrochloric acid concentrations as well as forming complexes with hydrofluoric acid [mainly for Zr(IV) and Nb(V)][192].

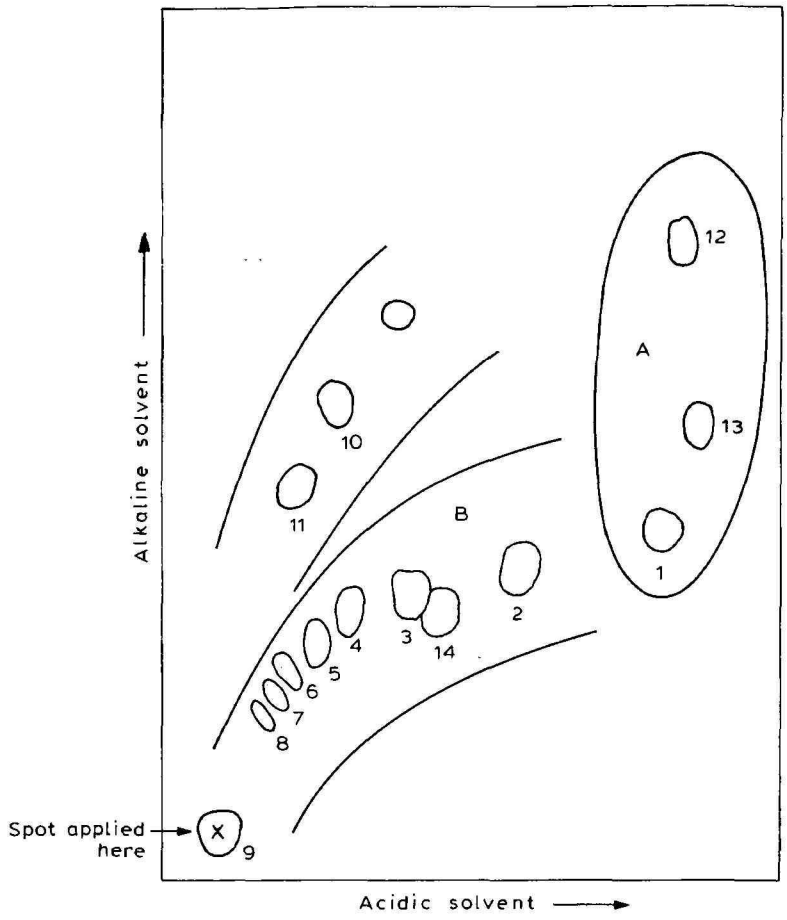


Fig. 21. Two-dimensional separation of oxyacids of phosphorus on paper. Alkalin solvent 1 (Ebel)–acidic solvent 3 (Grunze and Thilo). 1, orthophosphate; 2, pyrophosphate; 3, triphosphate; 4, tetraphosphate; 5, pentaphosphate; 6, hexaphosphate; 7, heptaphosphate; 8, octaphosphate; 9, Graham's salt; 10, trimetaphosphate; 11, tetrametaphosphate; 12, hypophosphite; 13, phosphite; 14, hypophosphate. Reproduced from ref. 191 with permission.

(2) It is also possible to separate in one direction by partition chromatography (butanol–2 *N* hydrochloric acid) and in the other by ion exchange (1 *N* aqueous magnesium chloride) on phosphorylated cellulose paper (Fig. 23). In the presence of hydrochloric acid (in the first dimension) the ion-exchange groups remain practically unionized and the metal ions move as on ordinary cellulose paper. The butanol–hydrochloric acid solvent cannot be removed entirely by evaporation and the remaining hydrochloric acid is neutralized with ammonia vapour[193].

4.11. Miscellaneous

Several reports have discussed the two-dimensional chromatography of organic acids on paper[5–7,194] and cellulose[195], of indole derivatives[196,197] and catechola-

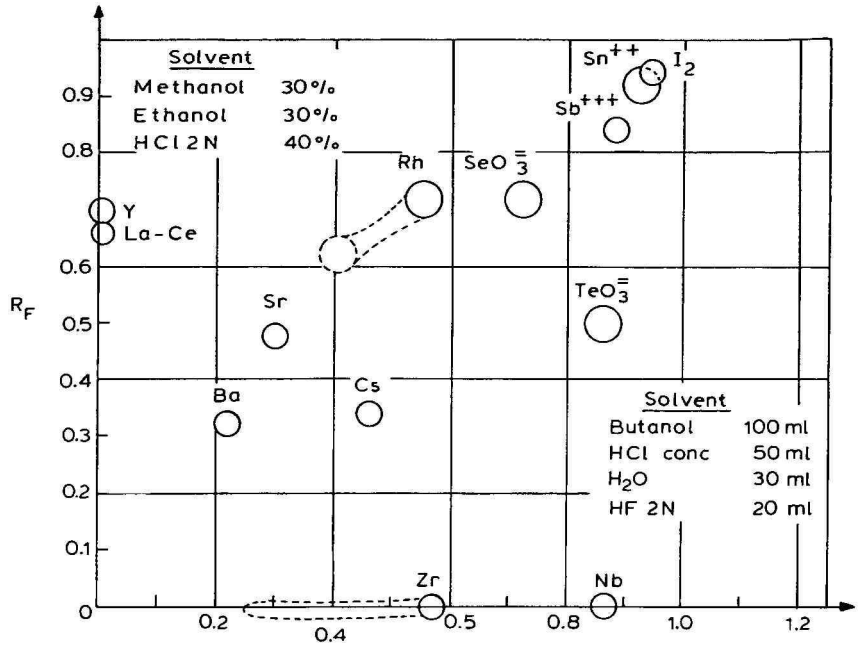


Fig. 22. A two-dimensional chart showing the distribution of the major fission products when chromatographed first with methanol–ethanol–2 *N* HCl (30:30:40) and then with butanol–conc. HCl–water–conc. HF (100:50:48:2). Reproduced from ref. 192 with permission.

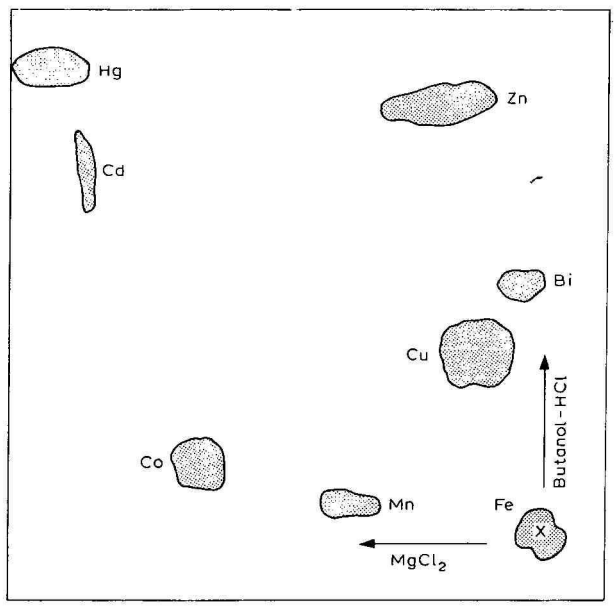


Fig. 23. Two-dimensional separation of metal ions on a 14-in. square of phosphorylated cellulose paper containing dihydrogen phosphate groups in the monoammonium salt form. Development is by the downward flow of the organic phase of a mixture of *n*-butanol saturated with 2 *N* HCl (partition chromatography) followed by 1 *N* magnesium chloride (ion-exchange chromatography). After the first run, the sheet is dried over ammonia to neutralize excess acid and to convert the paper to the original form. Reproduced from ref. 193 with permission.

TABLE 16

SEPARATION OF MISCELLANEOUS COMPOUNDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (in.)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
12	Organic acids	Paper (Durieux 122), 45 × 45 cm		Isopropanol–ammonia–water (70:5:25)	12 h, 35–40 cm	Hood	1-Propanol–eucalyptol–formic acid (50:50:20) + water until turbid	5 h, 35–40 cm	5
21	Organic acids	Paper (Whatman No. 1), 40 × 50 cm		Ethanol–ammonia–water (80:5:5)	14 h	8 h	1-Propanol–eucalyptol–formic acid (50:50:20) + water until turbid	14 h	6,7
14	Organic acids	Paper (Whatman 3MM)	3	*sec.*-Butanol–*n*-propanol–90% formic acid–water (75:25:100:48); after standing, use upper layer for development while lower layer saturates tank for 48 h prior to run	7 h	Dry, 12 h, wash with acetic acid, dry	*n*-Propanol–ammonia–water (1000:1.25:2.00)	9 h	194
8	Oxy acids	Cellulose MN 300 HR, 20 × 20 cm, 0.35 mm		Isopropanol–ethyl acetate–water (23.5:65:11.5)	14.5 cm		Formic acid–ethyl acetate–water (1:3:1)	14.5 cm	195
6	Indole derivatives	Si gel G 22, 20 × 10 cm, 0.3 mm, 20°C, 12 h		Isopropanol–25%–ammonia–water (20:1:2)			Butanol–acetic acid–water (15:3:5)		196
2	Indoleacetic and indolecarboxylic acids	Si gel G (Merck), 20 × 20 cm, 0.3 mm, 105°C, 20 min		Methyl acetate–isopropanol–ammonia (45:35:20)			Chloroform–acetic acid (95:5)		197

(*Continued on p. 184*)

TABLE 16 (*continued*)

SEPARATION OF MISCELLANEOUS COMPOUNDS

Column headings as in Table 1.

N	*Compounds*	*Stationary phase*	*SSP (in.)*	*Solvent 1*	*t/L*	*Drying*	*Solvent 2*	*t/L*	*Ref.*
5	Catecholamine metabolites	18% cellulose, 10 × 10 cm, 0.4 mm		Isopropanol–5% ammonia (4:1)	2 h		Benzene–acetic acid–water (146:73:2)	45 min	198
11	Dansylated derivatives of brain catecholamines and their derivatives	Kieselgel G		(a) Diisopropyl ether (b) Butyl acetate–triethylamine (100:20) (2 ×)			Triethylamine–diisopropyl ether (100:20) (2 ×)		120
11	N-Acetylated derivatives of biogenic amines	Kiesel G		(a) Ethyl acetate–butyl acetate (100:20) (b) Benzene–methanol (90:10) (2 ×)			Chloroform–triethylamine (100:20)	13 cm	120
20	Hypnotics (15 barbiturates, 3 bromoureides, phenytoin + glutethimide)	Si gel GF_{254}, 20 × 20 cm, 0.25 mm, 105°C, 30 min		Chloroform–diethyl ether (75:25)	10 cm		Isopropanol–chloroform–25% ammonia (45:45:10)	10 cm	199
3	Streptomycins	Si gel (Merck), 0.03 mm, 110°C, 60 min	5.0 cm away from cathode	2% Piperidine + 2% *p*-toluenesulphonic acid in water-saturated *n*-butanol	16 cm, 3.5 h		Electrophoresis with 1% $Na_2B_4O_7$ solution (pH 9.6), 300 V, 23–28°C	3 h	200
11	1,4-Benzodiazepine drugs (blood, urine)	Si gel G, 20 × 20 cm, 0.25 mm, 110°C, 30 min	1.5	Chloroform–benzene–diethyl ether (20:10:70)	10 cm		Benzene–acetone (90:10)		201, 202
15	Chlorpromazine and metabolites	Si gel (Brinkmann 254F), 0.25 mm, 100°C, 4 h	2	Acetone–methanol–methanolamine (100:30:1)	12 cm	42°C, 10 min	Isopropanol–ethanol–ammonia (2:1:1)	12 cm	203
14	Phthalodinitrites and related metabolites	(1) Si gel HF–cellulose (1:1) on 4 × 20 cm strip (2) Acetylated cellulose F layer, 15 × 20 cm		On (1): Carbon tetrachloride–ethyl acetate–acetic acid (7:2:0.5)	15 cm	Air, 20 min	On (2): Methanol–diethyl ether–water (7:2:0.5)	10 cm	204

4	Aflatoxins b_1, b_2, g_1, g_2 (figs)	Si gel 60, 105°C, 1 h		Toluene–ethyl acetate–90% formic acid (5:4:1)	17 cm	Dry, dark, room temp., 15 min	Acetone–chloroform (1:9)	17 cm	205
4	Aflatoxins (corn)	SILG-HR-25 (Brinkmann), 10 × 5 cm		Acetone–chloroform (12:88)	8 cm	Air stream	95% Denatured ethanol (Mallinckrodt 7006)	4.5 cm	206
37	Milk constituents from which aflatoxin Mi isolated	Si gel 60 (Merck), 20 × 20 cm, 0.2 mm		Chloroform–acetone–2-propanol (80:15:15)	10 cm		Toluene–ethyl acetate–90% formic acid (60:30:10)	10 cm	207
12	Carbonyl dinitrophenylhydrazones	MgO–Microcell T38 (1:1), 60°C, 1 h, 20 × 20 cm		Light petroleum–chloroform (85:35)	12 cm		(a) Chloroform-SVR (80:20) (2 ×) (b) 20% Carbowax 400 in chloroform (impregnates plates) (c) Rotate plate 180° and develop in PE		208 (Fig. 24)
5	Mixture of Ni(II) bis-diethyl- and bisdihexyl-dithiocarbamate complexes	Silufol Si gel (Kavalier), 15 × 15 cm, 120°C, 1 h		Chloroform–cyclohexane (3:4)	20 min		Chloroform–cyclohexane (3:4)		209
7	B_6 vitamers	Si gel H, 10 × 15 cm, 0.25 mm		Isoamyl alcohol–acetone–water–diethylamine (24:18:6:8)		Warm air	2-Butanol–ethanol–1.5 *N* ammonia–isoamyl alcohol–diethylamine (20:6:7:2:2)		210
12	1,3,5-Triamino-2,4,6-trinitrobenzene and its impurities	30 g Si gel G + 1 g Zn dust, 20 × 20 cm, 110°C, 2 h	1 in.	1,2-Dichloroethane	1 h	10 min	Acetone–light petroleum (1:9)	1	211

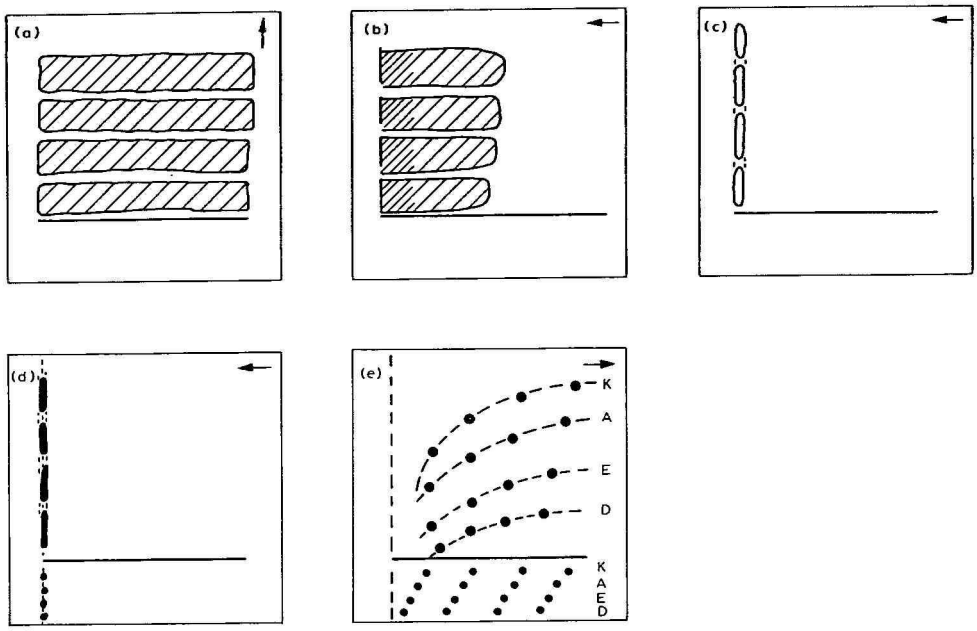


Fig. 24. Diagrammatic representation of the two-dimensional separation of dinitrophenylhydrazones (direction of solvent travel indicated by arrow). (a) Stage 1, class separation; (b) stage 2, first concentration; (c) stage 3, second concentration; (d) stages 4 and 5, impregnation and marker application; (e) stage 6, chain length separation. K = ketones; A = anals; E = enals; D = dienals. Reproduced from ref. 208 with permission.

mine metabolites[120,198] on silica and cellulose, of barbiturates[199], streptomycins[200], benzodiazepine[201,202] and chlorpromazine[203] drugs on silica and of phthalodinitriles[204] on a mixed plate, where a silica–cellulose strip had been coated at the side of an acetylated cellulose layer. In addition, aflatoxins[205–207], carbonyldinitrophenylhydrazones[208], dithiocarbamate complexes[209] and some B_6 vitamers[210] have also been resolved by two-dimensional TLC. Detailed chromatographic conditions for these separations are given in Table 16.

Craske and Edwards[208] developed an original two-dimensional technique for the separation of carbonyl dinitrophenylhydrazones (Fig. 24). Solutes were first resolved into different classes (alkanones, alkanals, alk-2-enals and alka-2,4-dienals) by adsorption, and next on the basis of chain length by partition. Whereas initial class separation required a small sample to prevent overloading, secondary chain length separation following Carbowax 400 impregnation required a large sample to facilitate solute detection. This problem was solved by streaking the sample across the width of the plate, developing in the first solvent and subsequently performing a chromatographic concentration step. Orthogonal elution in chloroform–SVR (80:20) concentrated the spots on one side of the plate. The layer was then impregnated with 20% Carbowax 400 in chloroform. The plate was rotated through 180° and chain resolution was effected by development in light petroleum.

5. CONCLUSION

In summary, two-dimensional TLC applications may be achieved using:

(1) a one-sorbent layer and solvents with different selectivity for the various solutes;

(2) a mixed-sorbent layer and eluents chosen such that one particular sorbent dictates retention in a given direction;

(3) coupled layers where two different sorbents are coated side-by-side, each effecting a separation according to a different retention mechanism;

(4) modification of the plate (impregnation) prior to the second development;

(5) derivatization of the solute prior to the second development;

(6) coupled separation techniques (TLC–GC, TLC–electrophoresis).

Sample purification may be achieved in one direction and separation in the other. The main advantage of the technique lies in its efficiency, as a large number of spots may be resolved on the chromatographic plate[21], provided that the initial spot size is small and the sample is not overloaded. In addition, widely different components may be resolved from a given mixture.

Perhaps the main disadvantages of a two-dimensional system are the serious difficulties encountered in quantitating a significant number of spots, the difficulties of predicting R_F values obtained from the second plate development, as these are generally affected by the previous elution, and the possible irregular ascent of the second solvent, leading to spot distortion. It is possible to correct for the latter problem, if not by selecting more "miscible" solvent systems, then by grafting two thin layers and transferring spots from one to the other prior to the second development[21,12]. As for the prediction of R_F values, a blank plate could be developed in the first eluent prior to spotting the various reference solutions and chromatography in the second direction.

Thus the problem of measuring compound concentrations remains the most critical, at least when working with non-radioactively labelled material or with compounds that cannot all react with a fluorescent or similar tag.

Nevertheless, this method is extremely powerful and rapid. With a total analysis time of about 1 h, a spot capacity well exceeding those currently achieved in conventional TLC or even HPLC can easily be obtained. The spot capacity of the figures reproduced above is in the range 150–300 (except in Fig. 15). We are of the opinion that this method or more generally bi- and tri-directional chromatographic techniques have considerable potential for the separation of complex mixtures; when there are a few ten to a hundred components to resolve, their use may save a considerable time in the selection of a convenient solvent mixture and/or chromatographic system allowing the complete separation in one HPLC run. If the mixture is more complex (several hundred components) they offer the only possibility of a simple, total analysis.

Accordingly, instrumentation for two-dimensional chromatography will be the subject of intense development work in the near future, and solutions will eventually be found for the problems discussed above.

6. SUMMARY

In view of the large spot capacity available, much larger than in conventional thin-layer chromatography (TLC), two-dimensional thin-layer chromatography is an extremely powerful and rapid separation technique. This paper presents a review of the literature up to early 1982 on the analytical applications of two-dimensional TLC classified according to the chemical nature of the compounds separated. Technical aspects of the method (single, mixed or coupled sorbent layers, plate impregnation, solute derivatization, coupling with other analytical techniques), together with effective mechanisms of solute retention are discussed. Available methods for spot detection and quantitation are reported. Future trends of two-dimensional TLC are commented. Over 200 references are cited.

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STATISTICAL APPROACH TO CHROMATOGRAPHIC THEORY

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CONTENTS

1. INTRODUCTION

The theoretical plate model continues to enjoy widespread popularity as a description of the behavior of chromatographic peaks. The plate model is generally attributed to Martin and Synge[1], but has been developed further and modified by Glueckauf[2], Mayer and Tompkins[3] and others. Giddings[4] gave an excellent discussion of the plate theory and its limitations.

In the plate theory of chromatography, a column is divided into a number of imaginary sections called plates. In each plate it is assumed that a sample substance is partitioned between the stationary and mobile phases and that equilibrium has been attained. Then the mobile phase in each plate moves forward to the next plate, carrying the sample substance in the mobile phase forward exactly one plate. A new partitioning occurs simultaneously in each plate, and it again is assumed that equilibrium is attained. This process is repeated many times, until sample constituents move along and off the column at different rates and thus are separated.

The number of imaginary sections in a column is generally called the number of theoretical plates, or theoretical plate number, and is designated as N (or n). The numerical value of N for any given column length is maximized by using very small spheres of uniform diameter, thinly coated with a stationary phase and carefully packed, as the column stationary phase. Factors such as column dimensions and

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fittings and proper eluent flow-rate also affect the value of N and hence the separation efficiency of the column.

There is no convenient way of measuring the intrinsic value of N; it must be calculated from measurable parameters, namely the retention time (or volume) of a peak and the peak width (or σ, which is a function of peak width). The defining equation for this calculation is

$$N = 16\left(\frac{t}{w}\right)^2 = \frac{t^2}{\sigma^2}$$

where t is the peak retention time, w is the peak width at its base (in the same units as t) and σ^2 is the variance of the peak width.

Some chromatographers prefer to use the number of effective theoretical plates as a measure of the separation power of a column:

$$N_{\text{eff}} = 16\left(\frac{t - t_0}{w}\right)^2 = \frac{(t - t_0)^2}{\sigma^2}$$

where t_0 is the retention time of a non-sorbed substance, or the "dead time" of the column. As early as 1959 Purnell[5,6] noted that N_{eff} (for which he used S, rather than N) is critical in determining the separation ability of a chromatographic column. He found that the resolution of alkanes was inconsistent with the observed value of N when the retention volumes are very small. Widely used equations show that resolution of chromatographic peaks is proportional to the number of effective theoretical plates.

The plate theory of chromatography has been criticized as lacking in physical reality because eluent flow in actual columns obviously is continuous and not a discontinuous flow from one plate to the next as portrayed by the plate theory. It is debatable whether this objection is valid because any theory that gives results consistent with experimental behavior would be useful despite differences in the actual and theoretical mechanisms.

Giddings[4] criticized the plate model on several counts and concluded that it "fails in the most important test of all —the very practical matter of predicting zone dispersion as a function of the numerous variables open to manipulation by the investigator". These variables include the particle size of the solid support, thickness of stationary phase coating, eluent flow-rate and diffusion coefficients in the stationary and mobile phases.

The rate theory of chromatography has tended to supplement, rather than replace, the plate theory. The Van Deemter equation[7] describes the effects of eluent flow-rate, longitudinal diffusion and multi-path effects within the column on plate height, H (H = column length, divided by N). For capillary columns in gas chromatography, the Golay equation[8] shows how diffusion coefficients, thickness of stationary phase coating, column diameter, flow-rate, etc., contribute to plate height, H. Giddings[4] has made major contributions to the dynamics of chromatography and has shown the effect of many experimental parameters on plate height in both gas (GC) and liquid chromatography (LC).

Although a theoretical value for H can be calculated from the diffusion coef-

ficients and other parameters contained in rate equations, the calculations often are not very accurate. For example, Desty and Goldup[9] compared experimental and calculated values for terms in the Golay equation and found good agreement for the B term but that the experimental C term was 2–6 times the calculated value. The major value of rate equations is in predicting in a qualitative manner (or semi-quantitative at best) how a change in particle size, for example, will affect chromatographic behavior.

Most chromatographers still rely on only two actual measurements to evaluate performance: peak retention time and peak width. The discussion in a recent book on liquid chromatography[10] is fairly typical of the way in which the dynamics of chromatography currently are handled. The authors consider that the theoretical plate number, N, of various chromatographic peaks is approximately constant and therefore they consider both N and H as measures of chromatographic efficiency. Thus, the rate theory and plate theory are in a way still tied together.

There seems to be some confusion as to how N varies (or does not vary) as the capacity factor, k, changes (recall that retention time of a peak varies directly with its capacity factor). While Snyder and Kirkland consider that N is approximately constant with k, Grob[11] states that N tends to increase with higher k and Kaiser[12] indicates that N decreases as k becomes larger. Jennings[13] provides a nice experimental answer to this question. Careful gas chromatographic separation of n-alkanes on a capillary column shows that N is very high at low values of k and decreases with increasing k, rapidly at first when k is small, and then more slowly at larger k values, eventually approaching an asymptotic value. Their data show that n_{eff} starts at or near zero and increases as k becomes larger. N_{eff} appears to approach the same asymptotic values as N. The change in N or N_{eff} with k is particularly great at k values below 1.0.

In this paper we derive simple statistical expressions for calculating the mean and variance of chromatographic peaks that are still on a column (position peaks) and for these peaks as they leave the column (exit peaks). The variances of position and exit peaks as a function of capacity factor, k, are compared. We also show how the major contributions to peak broadening in capillary column GC can be determined at any k value using gaseous diffusion coefficients computed from empirically determined constants for the atoms and chemical groups making up the carrier gas and the compounds separated. First, the peak variance contributions resulting from axial diffusion are calculated from a modified form of the Van Deemter equation and are subtracted from the measured peak variances. Then the remaining variance of each peak is plotted against a function of the capacity factor, k. A plate number is calculated from the slope of this linear plot which is independent of k and thus provides an excellent measure of performance for a column operating under specified, fixed conditions. The intercept of this plot provides an estimate of the extra-column peak broadening of the chromatographic system.

For both GC and LC columns run at a single flow-rate, a similar approach is outlined that gives another plate number that also is independent of k but which includes any peak broadening effects resulting from axial diffusion. This plate number is also useful in describing the separating ability of a column under fixed conditions and in predicting the variance of peaks of different k values from those in the test chromatogram.

The authors feel that the material presented here will correct some of the confusion or misconceptions that many chromatographers seem to have about plate theory. We also think that the approach presented is a simple but practical way of handling some of the dynamic effects that determine the variance of chromatographic peaks.

2. PLATE MODELS

Using a statistical approach, we shall study two classical models falling into the category of plate theories: the first is the discrete flow model and the second the continuous flow model. The characteristic feature of a plate model is that the chromatographic column is considered to be divided into a sequence of disjoint segments, or "plates". In our discussion, we shall refer to these as theoretical segments (abbreviated to TS). The sample molecules proceed from one TS to the next until they leave the last segment and exit from the column.

The purpose here is to derive statistical equations for the mean and variance of a peak that is still on the column (a position peak), and for a peak leaving the column (an exit peak); this will be done for each of the plate models. The statistical approach also leads to equations that describe the entire shape of position and exit peaks, although such equations for counter-current chromatography (CCC) are already available in the literature.

3. DISCRETE FLOW MODEL

The assumptions of the discrete flow plate model are (1) the entire mobile phase moves from each segment to the next at the end of discrete equal time intervals and (2) the sample chemical remains in equilibrium between the stationary and the mobile phases. In our analysis we shall study the movement of a single molecule through the column. In this form the equilibrium condition is expressed by the condition that the probability that the molecule is in the mobile phase is p, while the probability it is in the stationary phase is $1 - p$. Thus $p = \frac{1}{1 + k}$, where k is the well known capacity factor. Thus the position of the molecule is random and depends crucially on the random "decisions" on whether to stick in the stationary phase or be free in the mobile phase during a given time unit. We shall measure the passage of time by the number of transfers (n) of the mobile phase that have occurred. We shall measure the location of the molecule by noting which segment it is in. Two quantities are of particular interest: one is the probability distribution of the position of the particle at time n, and the other the probability distribution of the time when the molecule leaves the column (the exit time).

We shall first examine the position distribution. In each time period the particle either goes to the next segment of stays in its current segment. The first event takes place with probability p and the second with probability $1 - p$. Which of these two events actually occurs in the kth time interval can be represented by the random variable

$$B_k = \begin{cases} 1 \text{ with probability } p \\ 0 \text{ with probability } 1 - p \end{cases}$$

Random variables of this type are known as "Bernoulli" random variables[14]. If we assume that our molecule starts in segment zero at time zero, then its position at time n [denoted by $X(n)$] is

$$X(n) = \sum_{k=1}^{n} B_k$$

As the B_ks are random, $X(n)$ is also random. The Bernoulli random variables in the sum are all independent and identically distributed with mean p and variance $p(1 - p)$. It follows that the expected value of $X(n)$ is

$$E[X(n)] = E\left(\sum_{k=1}^{n} B_k\right) = \sum_{k=1}^{n} E(B_k) = np \tag{1}$$

and the variance of $X(n)$ is

$$\mathrm{Var}[X(n)] = \mathrm{Var}\left(\sum_{k=1}^{n} B_k\right) = \sum_{k=1}^{n} \mathrm{Var}(B_k) = np(1 - p) \tag{2}$$

These could also be written as

$$E[X(n)] = n\left(\frac{1}{1 + k}\right) \tag{3}$$

$$\mathrm{Var}[X(n)] = n\left[\frac{k}{(1 + k)^2}\right] \tag{4}$$

The central limit theorem of probability[14] tells us that $X(n)$ is asymptotically normal, *i.e.*, the distribution of $X(n)$ approaches closer and closer to a normal, or Gaussian, distribution as n increases ($n \approx 30$ is usually considered large enough for this to be a good approximation).

Probability theory will provide even more detailed information. An elementary result tells us that the sum of n independent identically distributed Bernoulli random variables with parameter p has a binomial distribution with parameters n and p (ref. 14). It follows that

$$P\{X(n) = j\} = \binom{n}{j} p^j (1 - p)^{n-j} = \frac{n!}{(n - j)!j!} \cdot p^j (1 - p)^{n-j}$$

$$= \frac{n!}{(n - j)!j!} \frac{k^{n-j}}{(1 + k)^n} \tag{5}$$

where j is some particular TS in the column and n is the number of transfers, or the

number of time intervals that have elapsed for a substance of capacity factor k. Eqn. 5 can be used to calculate the distribution of molecules along the various TS in a column by inserting various values of j into the equation. The result calculated will be the fraction of the molecules in each theoretical segment.

Next we examine the problem of determining the exit time distribution. If we denote the exit time by T, then $T = r + \sum_{k=0}^{r-1} D_k$. In this equation r is the number of theoretical segments in the column and therefore is the minimal amount of time necessary for the molecule to leave the column if it never enters the stationary phase. D_j is the (random) time that the molecule spends in the stationary phase of segment j. D_j can take on the values 0. 1, 2, ..., and it does so with probabilities p, $p(1 -)$, $p(1 - p)^2, \ldots$, respectively. This is the distribution of a geometric random variable with parameter p (ref. 14). Thus the random variables $D_j, j = 0, \ldots, r - 1$ are independent, identically distributed, geometric random variables with parameter p. The mean and variance of such a geometric random variable is $(1 - p)/p$ and $(1 - p)/p^2$, respectively. Thus we obtain

$$E(T) = E\left(r + \sum_{k=0}^{r-1} D_k\right) = r + \sum_{k=0}^{r-1} E(D_k) = r + r\left(\frac{1-p}{p}\right) = \frac{r}{p} = r(1 + k) \quad (6)$$

$$\mathrm{Var}(T) = \mathrm{Var}\left(r + \sum_{k=0}^{r-1} D_k\right) = \mathrm{Var}\left(\sum_{k=0}^{r-1} D_k\right) = \sum_{k=0}^{r-1} \mathrm{Var}(D_k) = r\left(\frac{1-p}{p^2}\right) = rk(1 + k) \quad (7)$$

We can once again apply the central limit theorem of probability to conclude that T is asymptotically normal, *i.e.*, as r becomes large the distribution of T approaches the normal distribution. It is even possible to obtain the exact probability distribution of T. To do this we utilize an earlier result: $P\{X(n) = j\} = \binom{n}{j} p^j (1 - p)^{n-j}$.
We obtain the following:

$P\{T = n\} = P\{X(n - 1) = r - 1$ and that the molecule is in the mobile phase in the next time interval$\} =$

$P\{X(n - 1) = r - 1\}\, P\{$mooecule is in mobile phase in next time interval $\} =$

$$[\binom{n-1}{r-1} p^{r-1} (1 - p)^{n-r}]\, p = \binom{n-1}{r-1} p^r (1 - p)^{n-r}$$

Thus

$$P\{T = n\} = \frac{(n-1)!}{(n-r)!(r-1)!} \cdot \frac{k^{n-r}}{(1+k)^n} \quad (8)$$

The result in eqn. 8 is the fraction of molecules of capacity factor k that leaves a column, containing r theoretical segments, during the nth time period.

4. CONTINUOUS FLOW MODEL

The basic assumptions of this model are as follows: (1) eluent flows at a constant rate from one segment to the next; (2) the mobile and stationary phases remain in equilibrium at all times; and (3) there is perfect mixing in the segments. As we shall be looking again at only a single molecule, we interpret condition (2) to mean that the probability that the molecule is in the mobile phase at any given time is $\frac{1}{1+k}$ and the probability that it is in the stationary phase is $\frac{k}{1+k}$. "Units" are set up as follows. The amount of eluent in one segment is one unit of volume. The amount of time it takes for one unit volume to flow from one segment to the next is defined to be one time unit. Thus, in a time interval Δt, an amount of eluent Δt flows from each segment to the next.

Suppose we have r segments (numbered 0, 1, ..., $r-1$). Looking at some molecule of sample as it moves through the segments, we see that:

(1) It spends a random amount of time, D_i, in segment i.

(2) These "delay times", D_i, are independent, identically distributed random variables.

(3) The exit time for the molecule is $\sum_{i=0}^{r-1} D_i$.

(4) The TS the molecule is in at time t, $N(t)$, is given by

$$N(t) = \left\{\text{minimum value of } n \text{ such that } \sum_{i=0}^{n-1} D_i \leqslant t < \sum_{i=0}^{n} D_i\right\} \tag{9}$$

(Note the above D_i is not to be confused with the one used in the discrete flow model.)

Clearly, our first task must be to determine the distribution of the random variables, D_i. To do this we look at a single segment. We wish to calculate the probability that a molecule (which is in this segment) leaves the segment in the next time interval Δt (Δt is assumed to be small). For this to happen it is necessary that the molecule (a) be in the mobile phase, and (b) be in that particular Δt volume of eluent that is leaving. This probability is

$$P\{a\} \cdot P\{b\} = \left(\frac{1}{1+k}\right)\left(\frac{\Delta t}{1}\right) = \Delta t\left(\frac{1}{1+k}\right)$$

This result is characteristic of an exponential delay time with parameter $\lambda = \frac{1}{1+k}$ (ref. 14). The density of such a random variable is $\lambda e^{-\lambda t}$ ($t \geqslant 0$).

With this piece of information together with some standard results of probability theory, we can now determine the exit time density and the probability distribution of the molecules' position at time t. First, the distribution of the exit time is the distribution of the sum of r independent identically distributed exponential random

variables. It is known that this distribution is a gamma distribution with parameters r and λ (ref. 14). The density function is

$$f(t) = \frac{\lambda(\lambda t)^{r-1} e^{-\lambda t}}{(r-1)!} \quad (t \geqslant 0)$$

Now we use the fact that the mean and variance of our exponential random variables are $1/\lambda$ and $1/\lambda^2$ respectively. Let T denote the exit time [which will have the density $f(t)$ above]. Then:

$$E(T) = E\left(\sum_{i=0}^{r-1} D_i\right) = \sum_{i=0}^{r-1} E(D_i) = \frac{r}{\lambda} = r(1+k) \tag{10}$$

$$\mathrm{Var}(T) = \mathrm{Var}\left(\sum_{i=0}^{r-1} D_i\right) = \sum_{i=0}^{r-1} \mathrm{Var}(D_i) = \frac{r}{\lambda^2} = r(1+k)^2 \tag{11}$$

Once again we can apply the central limit theorem to conclude that the distribution of T is asymptotically normal (as $r \to \infty$).

It will be noted that the mean exit time (eqn. 10) is the same for both models but that the variance of the exit peak is $r(1+k)^2$ for the continuous flow model and $rk(1+k)$ for the discrete flow model.

To obtain the distribution of the position of sample molecules at time t, we note from eqn. 9 that D_i being identically distributed random variables makes $N(t)$ a Poisson process with parameter λ (ref. 15) [for the definition of $N(t)$, see eqn. 9]:

$$P\{N(t) = k\} = \frac{(\lambda t)^k e^{-\lambda t}}{k!} \tag{12}$$

for $k = 0, 1, \ldots, r-1$.

It can be shown by a slightly more sophisticated application of the central limit theorem that the distribution of $N(t)$ is asymptotically normal (as $t \to \infty$) (this result also requires that r be large enough that the molecule will not yet have left the column at values of t large enough to yield a good normal approximation).

5. THEORETICAL PLATE NUMBERS IN THE TWO MODELS

The theoretical plate number, N, and the effective theoretical plate number, N_{eff}, are of course widely used in chromatography. These may be defined by

$$N = \frac{[E(T)]^2}{\mathrm{Var}(T)} \tag{13}$$

and

$$N_{\mathrm{eff}} = \frac{[E(T) - t_0]^2}{\mathrm{Var}(T)} \tag{14}$$

where t_0 is the exit time for a non-sorbed substance and $E(T)$ is the expected exit time for a sample substance.

We can use the result we have obtained to calculate these quantities for both the discrete flow and continuous flow models. For the discrete flow mode:

$$N = \frac{[E(T)]^2}{\mathrm{Var}(T)} = \frac{[r(1 + k)]^2}{rk(1 + k)} = r\left(\frac{1 + k}{k}\right) \tag{15}$$

$$N_{\mathrm{eff}} = \frac{[E(T) - t_0]^2}{\mathrm{Var}(T)} = \frac{(rk)^2}{rk(1 + k)} = r\left(\frac{k}{1 + k}\right) \tag{16}$$

For the continuous flow model:

$$N = \frac{[E(T)]^2}{\mathrm{Var}(T)} = \frac{[r(1 + k)]^2}{r(1 + k)^2} = r \tag{17}$$

$$N_{\mathrm{eff}} = \frac{[E(T) - t_0]^2}{\mathrm{Var}(T)} = \frac{(rk)^2}{r(1 + k)^2} = r\left(\frac{k}{1 + k}\right)^2 \tag{18}$$

Thus, only in one of the four cases is the plate number result independent of k.

6. SOME CONSEQUENCES OF THE DISCRETE FLOW MODEL

In the discrete flow model the mean and variance of the location, $X(n)$, are expressed in units involving TS (here theoretical segments indicate the *position* of the molecule). On the other hand, the mean and variance of the exit time, T, must be expressed in time units. The fundamental time unit is the time needed for eluent to flow from one TS to the next. We wish to show that simple unit conversions can be used to relate results for peak locations to those for peak exit times. We define T_j as the time when a sample molecule enters the jth theoretical segments (note that $T_r = T$). Reasoning by analogy with eqns. 6 and 7, we have $E(T_j) = j(1 + k)$ and $\mathrm{Var}(T_j) = jk(1 + k)$. Using eqns. 3 and 4 to calculate $E[X(n)]$ and $\mathrm{Var}[X(n)]$ when $n \approx j(1 + k)$:

$$E[X(n)] = j(1 + k)\cdot\frac{1}{1 + k} = j \tag{19}$$

$$\mathrm{Var}[X(n)] = j(1 + k)\cdot\frac{k}{(1 + k)^2} = j\cdot\frac{k}{1 + k} \tag{20}$$

Now we see that $E(T_j) = E[X(n)](1 + k)$ and $\mathrm{Var}(T_j) = \mathrm{Var}[X(n)](1 + k)^2$. In other words, we can convert between means and variances of position and exit time random variables simply by multiplying by the conversion fact $(1 + k)$ for the means and $(1 + k)^2$ for the variances.

Counter-current chromatography (CCC) is a good system for illustrating the practical results of the equations derived. In CCC the solute molecules attain equilibrium between the mobile and stationary phases prior to each transfer to the next tube in the series. Thus, each tube is by definition a theoretical plate, according to the plate theory of chromatography, or a theoretical segment in our nomenclature. It has been recognized by several authors that CCC also is a reasonable model for explaining elution behavior in column chromatography, provided that axial diffusion, multipaths and other factors that contribute to peak broadening in column chromatography, but which are non-existent in CCC, are also taken into account. This will be done in the next section, but first let us consider only the peak broadening resulting from inter-phase broadening effects, with CCC as a model.

Fig. 1 shows the distribution of a solute along the series of 36 tubes ($r = 36$) in a CCC apparatus as a function of the number of transfers, n. The peaks were plotted for $k = 1.5$ from eqn. 5 with the aid of a programmable calculator. Note that the peak has become well defined and approximately Gaussian after only a few transfers and that the peak broadens and decreases in height as it moves along the series of tubes. Fig. 2 shows the same peak, calculated from eqn. 8, as it leaves the CCC apparatus and passes through an imaginary detector. The peak that was symmetrical in its position distribution of molecules now has a distinct tail. The explanation for this is that the latter part of the peak continues to broaden after the earlier portions have left the "column". This effect is of some significance because it demonstrates that in columns of low "performance" some peak tailing is predicted mathematically and is not necessarily caused by a poorly functioning column.

The tailing of an exit peak decreases and the peak becomes more Gaussian as the number of theoretical segments (r) in a column becomes larger. The tailing, or skewness, of a peak is predicted by the following equation:

$$\text{Coefficient of skewness} = \frac{1}{\sqrt{r}} \cdot \frac{2k^2 + 3k + 1}{(k + 1)^2[k/(k + 1)]^{1/2}} \tag{21}$$

(see ref. 14 for a definition of the coefficient of skewness). The second term in this equation has a value of just over 2 from $k = 1$ to $k = 10$, but increases rapidly as the value of k becomes very small.

It is well known that later eluting peaks are much broader than those with shorter retention times. From the exit peak variance (eqn 7) it will be seen that the peak width (4σ) is proportional to $\sqrt{k(1 + k)}$ and thus increases in approximately linear fashion with k (except at very low values of k). It is interesting to compare this with the way the width of a peak still on a column varies with k. This may be done by calculating the peak widths when the peak maximum is located in the jth theoretical segment in a column containing r theoretical segments. We shall choose j to be near the end of the column, say $j = 0.9\,r$. From eqn. 20 for the variance of a position peak we see that $4\sigma = 4\left[\frac{jk}{1 + k}\right]^{1/2}$. In Table 1 we see that the widths of peaks centered at j vary only slightly with increasing k, much less than the exit peaks (of course it takes longer for peaks of higher k to arrive at j). The reason that elution peaks are so much broader when k is high is that such peaks are moving more slowly and take longer to pass through the detector.

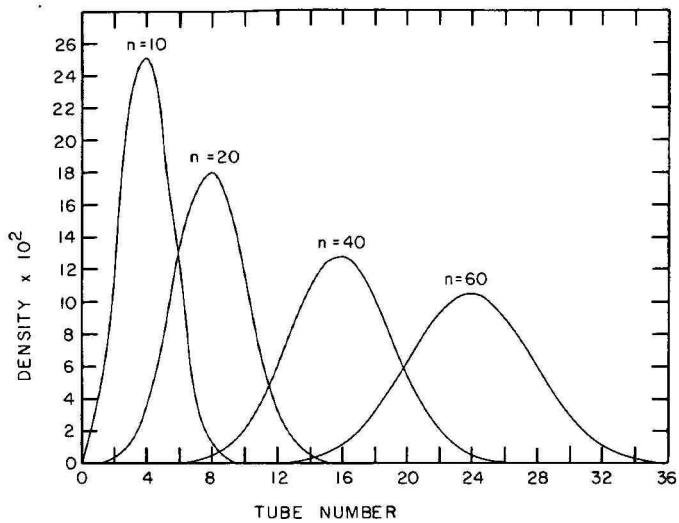

Fig. 1. Position peaks for a compound with $k = 1.5$ in a CCC apparatus of 36 tubes after n transfers.

Exit peaks calculated for the discrete flow model using eqn. 8 emphasize a major drawback of the plate theory that has been so widely used in chromatography. In no case does either N or N_{eff} (calculated from eqns. 13 and 14) agree with the actual number of plates (tubes) in CCC, which is r. The correct values for N and N_{eff} are given by eqns. 15 and 16, respectively. Fig. 3 shows the expected values of N and N_{eff} as a function of k, calculated from eqns. 15 and 16 for a CCC apparatus where $r = 1000$. The values of N are very high as $k \rightarrow 0$ and become meaningless as a measure of separating power. Similarly, a single value of H (height equivalent to a theoretical plate) is an ambiguous expression of column efficiency when H varies so widely for different peaks.

The application of eqns. 5 and 8 to CCC is well documented and there would seem to be little doubt as to their correctness. It is logical that eqns. 3–8 should apply also to column chromatography. An examination of actual column chromatograms is now in order, to determine whether the equations do or do not apply.

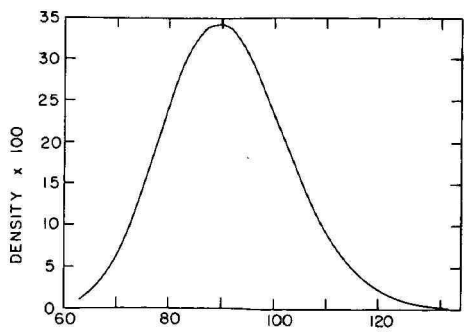

Fig. 2. Exit peak for a compound with $k = 1.5$ from a CCC apparatus of 36 tubes (n = number of transfers).

TABLE 1

WIDTHS (4σ) OF POSITION AND EXIT PEAKS AS A FUNCTION OF k

k	*Position width** (TS)	*Exit width*** (TS)	*Exit width**** (sec)
0.1	36	42	2.5
0.2	49	62	3.7
0.4	64	95	5.7
0.6	74	124	7.4
0.8	80	152	9.1
1.0	85	179	10.7
1.5	93	245	14.7
2.0	98	310	18.6
3.0	104	438	26.3
4.0	107	566	33.9
6.0	111	820	49.2
8.0	113	1073	64.4
10.0	114	1327	79.6
15.0	116	1960	117.6

* Calculated from $4\sigma = 4\left[\frac{jk}{1+k}\right]^{1/2}$, where $j = 900$.

** Calculated from $4\sigma = 4[rk(1+k)]^{1/2}$, where $r = 1000$.

*** Calculated from the previous column for an eluent flow-rate of 16.67 TS/sec.

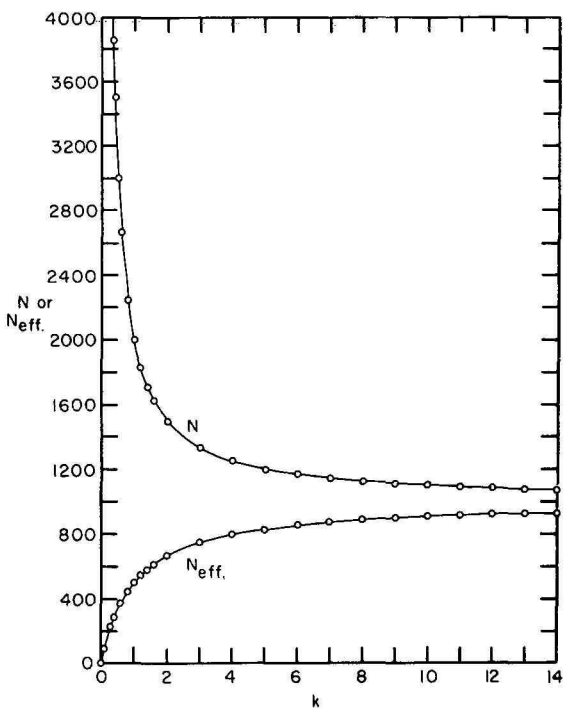

Fig. 3. Expected values of N and N_{eff} for an exit peak from a CCC apparatus where $r = 1000$.

7. CALCULATION OF PLATE NUMBERS FROM CHROMATOGRAPHIC DATA

When working with actual data for column chromatography, it is necessary to consider the various dynamic effects that contribute to the width of chromatographic peaks. The major effect almost always is what is termed "resistance to mass transfer", which we shall call "inter-phase broadening". Additional peak broadening occurs through axial diffusion, multi-paths (in packed columns) and extra-column effects such as broadening in fittings, connecting tubing and the detector. Injection band broadening is apt to be significant also, as was recognized by Keulemans as early as 1959[16,17].

If we assume that these broadening effects act independently of one another, the measured peak variance is the sum of the variances of the individual broadening effects. For capillary GC columns (where there is no multi-path effect), we can write

$$\sigma^2 = \sigma_{ec}^2 + \sigma_d^2 + \sigma_{ip}^2 \tag{22}$$

where ec stands for extra column, d for diffusion and ip for inter-phase. The approach taken will be first to estimate the peak variance resulting from axial diffusion and to subtract this from the measured peak variance. Then a plate number representing the inter-phase broadening can be calculated from the slope of a plot of the remaining peak variance against $k(1 + k)$, which comes from the peak variance in the discrete model, $rk(1 + k)$.

7.1. *Diffusion broadening*, σ_d^2

The effect of diffusion on plate height, H, is given by the Van Deemter equation, which has the form, $H = \frac{B}{u} + Cu$, where B is the diffusion term, u is the linear column flow-rate and C is the resistance to mass transfer. In this equation, $B = 2D_g$, where D_g is the axial diffusion coefficient in the gas phase (cm^2/sec).

According to the classical definition of H and N, the diffusion contribution to H is converted to σ_d^2 as follows:

$$H = \frac{L}{N} = \frac{L\,\sigma_d^2}{[t_0(1 + k)]^2} = \frac{2D_g}{u} \tag{23}$$

$$\sigma_d^2 = \frac{2D_g}{u} \cdot \frac{(t_0)^2\,(1 + k)^2}{L} = \frac{2D_g L(1 + k)^2}{u^3} \tag{24}$$

where L is the column length (cm) and u is the linear flow-rate (cm/sec).

One way to estimate the diffusion broadening variance is to run a chromatogram at two different flow-rates. Diffusion broadening varies as the inverse cube of the flow velocity, but inter-phase broadening varies only as the inverse of the flow velocity. This difference allows us to solve for diffusion broadening by solving two simultaneous equations (the dependence of the broadening on flow velocity will be considered in the next section).

Although this method works, a more convenient way is to use the method for

estimating gaseous diffusion coefficients proposed by Giddings[18]:

$$D_g \text{ (for A,B)} = \frac{10^{-3}T^{1.75}\left(\frac{1}{M_A} + \frac{1}{M_B}\right)^{\frac{1}{2}}}{p[(\Sigma_A v_i)^{1/3} + (\Sigma_B v_i)^{1/3}]^2} \tag{25}$$

where M_A and M_B are the molecular weights of the carrier gas and a chromatographically separated substance, respectively, T is the temperature (°K) p is the pressure (bar) and v_i are empirically determined values for various atoms and groups making up the carrier gas and the separated chemical. Giddings and co-workers obtained excellent agreement (usually to within $\pm 5\%$) between D_g values calculated this way and experimentally reported values[18].

As will be shown by an actual example, we found that this method gives reasonable results when applied to column chromatography. Although the values of D_g decrease as one proceeds to increasingly higher members of a homologous series, the fact that the D_g values are multiplied by $(1 + k)^2$ means that σ_d^2 (in sec^2) actually increases as one proceeds to later eluting peaks. Despite differences in individual D_g values, a linear regression plot of calculated σ_d^2 *versus* $(1 + k)^2$ is generally obtained with a high correlation coefficient.

7.2. *Inter-phase broadening*, σ_{ip}^2

The general approach taken is to subtract σ_d^2 from the measured variance of each peak and to plot the difference, σ_{net}^2, against one of the expressions for stochastic peak variance derived earlier. This should give a straight line with a slope related to a plate number and an intercept indicative of extra-column peak variance.

However, one question is whether $rk(1 + k)$ in the discrete flow model or $r(1 + k)^2$ in the continuous flow model is correct. For many plots, both give straight lines by linear regression. This is because the ratio of$(1 + k)^2/k(1 + k)$ does not change greatly with k at higher k values (say 2.5–15) and also that linear regression is insensitive to points of lower k that might not lie on a straight-line plot.

However, C values calculated from the Golay equation where several of the k values are quite low shows that slopes of individual points (y/x for each point) are nearly constant for plots of σ^2 *versus* $k(1 + k)$ but they vary considerably for the same k values when σ^2 is plotted *versus* $(1 + k)^2$. This supports the contention that the discrete flow is correct for column chromatography and that it is correct to plot σ^2 *versus* $k(1 + k)$ for inter-phase broadening.

Using eqn. 7 and making use of the conversion factor t_0/r (sec/TS) it can be shown that

$$\sigma_{ip}^2 = \frac{(t_0)^2\, k(1 + k)}{r} = \frac{L^2\, k(1 + k)}{u^2 r} \tag{26}$$

where L is the column length (cm), u is the linear flow-rate (cm/sec) and r is the number of theoretical segments in the column at the flow-rate employed. However, we know that the plate number, r, is proportional to the reciprocal of linear flow-rate.

Introducing a plate number, r', which is the number of theoretical segments in a column at u = 1cm/sec:

$$r = \frac{r'}{u}$$

$$\sigma_s^2 = \frac{L^2\, k(1 + k)}{u\, r'} \tag{27}$$

This equation for peak variance due to stochastic broadening was tested on data published by Kaiser and Rieder[19] for the separation of alkanes and aliphatic esters by capillary column GC at six different flow-rates. First, the peak variance resulting from axial diffusion was subtracted from the measured peak variance as outlined above. Then the remaining variance (σ_{net}^2) was plotted against $k(1 + k)$ and the plate number r' calculated from the slope of the straight-line plot obtained. A sample calculation is shown in Table 2. The results are summarized in Table 3, which shows a constant value for r' within a reasonable experimental error. The plate number, r, at any flow-rate can be calculated simply by dividing r' by u.

The plate number, r', seems to be a convenient way of evaluating and comparing column performances. It is computed easily from measured peak variances using linear regression and is independent of peak capacity factor. It is also independent of axial diffusion effects. This is good because diffusion really has nothing to do with the separating ability of a column other than contributing to the broadening of peaks. In some respects r' is similar to the C term in the Van Deemter and Golay equations. However, C is different for each peak whereas r' is not. It would appear that r' can be more easily and accurately measured from ordinary chromatographic data than can C.

At a fixed flow-rate it is convenient to obtain a plate number that includes

TABLE 2

SAMPLE DATA FROM KAISER AND REDIER[19] FOR t_0 = 146 sec SHOWING AXIAL DIFFUSION CONTRIBUTION TO PEAK VARIANCE

σ^2 (diffusion) was calculated from eqn. 24 using D_g values calculated from eqn. 25 at an estimated pressure of 1.2 bar. The values of the gaseous diffusion coefficient (D_g) used ranged from 0.0795 for C_9 to 0.0653 for C_{13}.

*Compound**	*k*	*σ^2 (measured) (sec^2)*	*σ^2 (diffusion) (sec^2)*	*σ^2 (net) (sec^2)*
C_9	1.26	1.52	0.63	0.88
E_9	1.45	1.96	0.74	1.22
C_{10}	2.38	4.15	1.33	2.82
E_{10}	2.75	4.88	1.64	3.24
C_{11}	4.51	10.41	3.38	7.03
E_{11}	5.23	13.34	4.32	9.02
C_{12}	8.55	35.34	9.65	25.69
E_{12}	9.94	43.88	12.66	31.22
C_{13}	16.2	112.7	30.0	82.7

* C = *n*-alkane and carbon number; E = alkane ester and carbon number.

TABLE 3

PLATE NUMBER (r') CALCULATED FROM DATA OF KAISER AND RIEDER[19] AFTER SUBTRACTING DIFFUSION PEAK VARIANCE

t_0 (sec)	u (cm/sec)	$r' \cdot 10^5$ (TS)
276	7.25	9.19
154.4	12.95	10.40
146.0	13.70	9.86
106.8	18.73	10.71
88.2	22.68	9.53
87.4	22.88	9.82
	Average:	9.92 (s = 0.56)

broadening resulting from axial diffusion as well as inter-phase peak broadening. This can be done simply by measuring the variance of each of the chromatographic peaks and plotting measured σ^2 against peak variance, $k(1 + k)$. The apparent plate number, r, is obtained from the slope of the linear plot. The intercept is indicative of the extra-column peak broadening plus the diffusion broadening of a non-sorbed or a very slightly sorbed peak.

This simple plotting method works because a plot of σ_d^2 *versus* $(1 + k)^2$ is linear and a plot of σ_d^2 *versus* $k(1 + k)$ is almost linear. The flow-rates that are normally used in chromatography sufficiently fast that diffusion contribution to peak width usually is not very substantial. Thus, any slight non-linearity of the σ_d^2 part of the plot is insignificant.

The equation relating measured peak variance to r and k is derived by converting the peak variance, $rk(1 + k)$, from TS units to sec^2 by dividing $\frac{r^2}{(t_0)^2}$ (t_0 is the hold-up time):

$$\sigma_{ip}^2 = \frac{rk(1 + k)}{r^2/(t_0)^2} = \frac{(t_0)^2}{r}[k(1 + k)] \tag{28}$$

where σ_{ip}^2 and t_0 are now in minutes or seconds. Substitution into eqn. 22 gives

$$\sigma^2 = \frac{(t_0)^2}{r} \cdot [k(1 + k)] + \sigma_{ec}^2 \tag{29}$$

where σ, t_0 and σ_{ec} are in minutes or seconds. This equation predicts that a plot of σ^2 *versus* $k(1 + k)$ for the various peaks in a chromatogram will give a straight line with slope $(t_0)^2/r$ and intercept $= \sigma_{ec}^2$.

The validity of eqn. 29 was tested on a number of actual chromatograms. Usually the chart speed of the recorder was 4–10 cm/min to facilitate measurement of the peak widths with a ruler and magnifying lens. The peak variance was obtained from the peak width at half of its height, $w_{1/2}$ (where $\sigma = 2.355\ w_{1/2}$) in order to minimize the effect of any tailing in the lower part of the peak.

Data for five chromatographic separations are summarized in Table 4. Chro-

TABLE 4

CALCULATION OF r FROM CHROMATOGRAPHIC DATA

Chromatogram	*Peak*	k	$k(1 + k)$	σ^2	*Results*
(A) n-Alkanes	C_7	0.14	0.16	0.00032 (min^2)	Correlation coefficient = 0.9999
by capillary	C_8	0.8	1.44	0.00090	$\sigma_2^2 = 0.00001$
GC^{13}	C_9	1.4	3.36	0.00187	Slope = 0.00518
t_0 = 9.72 min	C_{10}	2.3	7.59	0.00380	r = 182,500
Oven at 130°C	C_{11}	3.9	19.1	0.0096	
	C_{12}	6.5	48.8	0.0249	
	C_{13}	10.8	127.4	0.0661	
(B) n-Alkanes	C_8	0.97	1.91	$4.62 \cdot 10^{-5}$ (min^2)	Correlation coefficient = 0.9999
by capillary	C_9	2.31	7.65	$14.1 \cdot 10^{-5}$	$\sigma_2^2 = 2.27 \cdot 10^{-5}$
GC at two	C_{10}	5.42	34.8	$62.8 \cdot 10^{-5}$	Slope = $1.676 \cdot 10^{-5}$
different	C_{11}	12.33	164.4	$277 \cdot 10^{-5}$	r = 85,900
temperatures*.	C_8	0.60	0.96	$4.06 \cdot 10^{-5}$	
First set,	C_9	1.44	3.51	$7.21 \cdot 10^{-5}$	
60°C;	C_{10}	3.26	13.9	$26.0 \cdot 10^{-5}$	
second set	C_{11}	7.19	58.9	$101 \cdot 10^{-5}$	
70°C.					
t_0 = 1.20 min					
(C) Carboxylic	Acetic	1.8	5.04	0.0451 (mm^2)	Correlation coefficient = 0.9998
acids by	Propionic	3.4	15.0	0.0649	$\sigma_2^2 = 0.0348$
packed-column	Isobutyric	5.0	30.0	0.0909	Slope = 0.00196
GC**.	n-Butyric	6.55	49.4	0.1303	r = 2040
t_0 = 2.0 mm	Isovaleric	9.7	104	0.2426	
	n-Valeric	13.3	190	0.4057	
(D) Alkali	Li^+	4.35	23.26	51.8 (sec^2)	Correlation coefficient = 0.9988
metal ions	Na^+	6.10	43.2	83.0	$\sigma_2^2 = 19.0$
by ion	NH_4^+	8.47	80.1	148.0	Slope = 1.514
exchange***.	K^+	11.45	142.6	229.8	r = 1190
50-μl sample.	Rb^+	13.0	182.0	295.8	
t_0 = 42.5 sec					
(E) Alkali	Li^+	4.90	28.88	54.6 (sec^2)	Correlation coefficient = 0.9979
metals by	Na^+	6.54	49.30	62.4	$\sigma_2^2 = 16.3$
ion exchange.	NH_4^+	9.44	98.47	117.2	Slope = 1.067
20-μl sample.	K^+	12.51	169.0	200.0	r = 1430
t_0 = 39 sec	Rb^+	14.43	222.7	253.6	
(F) Pesticides	Sevin	0.955	1.87	0.000357 (min^2)	Correlation coefficient = 0.9996
by liquid	Prolate	1.16	2.50	0.000391	$\sigma_2^2 = 2.11 \cdot 10^{-4}$
chromatog-	Ruelene	1.72	4.67	0.000786	Slope = $0.7445 \cdot 10^{-4}$
raphy. t_0 =	Coral	1.94	5.72	0.000612	r = 2660
0.445 min §	Dursban	3.45	15.35	0.001356	
	trans-Permathrin	5.81	39.55	0.003236	
	cis-Permathrin	6.80	53.01	0.004100	

* J. Kaczvinsky, unpublished results (1981).

** Data from chromatogram in an advertising brochure (1981).

*** G. Sevenich, unpublished results (1981).

§ L. Rice, unpublished results (1981).

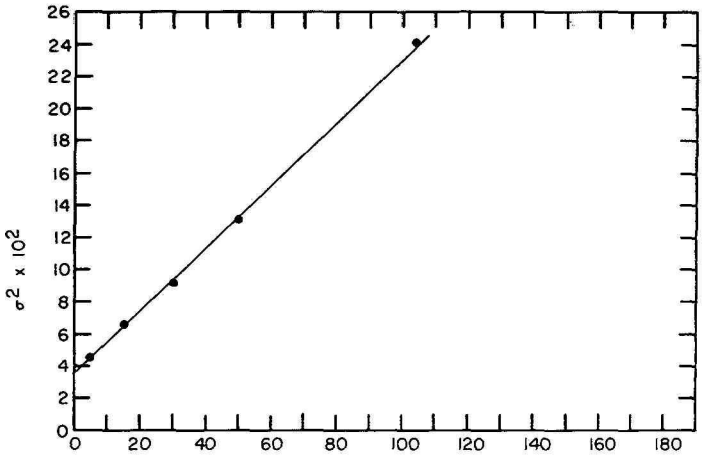

Fig. 4. Linear regression plot for chromatogram C in Table 2.

matogram A is unique among those tested in that the intercept, σ^2_{ec}, was essentially zero. Of course there is some error in measuring k and σ^2 for each peak, but the equipment and technique used were both known to be excellent.

The data for B in Table 4 are for two chromatograms run at different temperatures, yet all eight points lie on a straight line within reasonable experimental error. The intercept, σ^2_{ec}, is significant in this instance and constitutes nearly 50% of the measured variance of the first C_8 peak. Note that the early peaks are far more affected by σ^2_{ec} than the latter ones if the actual peak widths (4 σ) are compared.

Chromatogram C was run on a packed GC column and shows a far greater σ^2_{ec} relative to the measured peak variances than the chromatograms or capillary columns. Fig. 4 confirms that the experimental points actually do fall on a straight line when plotted according to eqn. 29. It is interesting to calculate the traditional plate number, N, before and after subtraction of σ^2_{ec} from σ^2 for each peak. Before any correction is applied, N increases from peaks 1 to 6: N = 695, 1190, 1580, 1750, 1890, 2020. After subtracting σ^2_{ec} from the variance of each peak, N decreases from peaks 1 to 6: N = 3050, 2570, 2390, 2200, 2200.

Chromatograms D and E are for an ion-exchange separation of alkali metal ions. Again, the data support the validity of eqn. 28 even though some of the peaks were tailed, and accurate measurement of peak width was difficult. The intercept, σ^2_{ec}, is smaller and the value of r is larger when the sample volume is reduced from 50 to 20 μl.

Chromatogram F in Table 4 was obtained with a commercial liquid chromatograph with a 10 cm × 4.6 mm I.D. column. The large value for r confirmed the excellent separating ability of the column, but the additional broadening represented by σ^2_{ec} was large. Much of this can be attributed to the use of a small "guard" column filled with a coarser reversed-phase absorbent than that used in the chromatographic column. Subsequent replacement of the guard column with a pre-column of slightly smaller diameter packed with 10-μm absorbent reduced σ^2_{ec} by almost 50%.

While there is no direct proof that the intercept, σ^2_{ec}, of our linear regression analysis gives an accurate measure of the sum of in-column and extra-column broad-

ening that applied equally to all peaks, the underlying principle does appear sound and the results obtained from actual data are reasonable. The idea of linear regression analysis of chromatographic data originated with Kaiser and co-workers[19–21], who plotted $w_{1/2}$ against k. They obtained the "real" number of theoretical plates from the slope and an indication of the extra-column peak broadening from the intercept. We think that the concept pioneered by Kaiser and co-workers is a valuable one but that their method of plotting the data is not completely correct. According to Guiochon[22], a plot of $w_{1/2}$ *versus* k is not linear at all values of k and the intercept of such a plot underestimates the "extra-column" peak broadening.

Smuts *et al.*[23] proposed a plot of peak variance against $(1 + k)^2$, although the purpose of this work was different from ours. This type of plot would follow if the continuous flow model [where the peak variance is $(1 + k)^2$] is correct for column chromatography. However, Smuts *et al.*[24] stated that such a plot is not completely linear. Plots of σ^2 *versus* $(1 + k)^2$ for the data in Table 2 also did not give a completely straight line, although the intercept was often not greatly different from that obtained when using the discrete flow model. All of our results suggest that the discrete flow model is better for column chromatography.

8. SUMMARY

The classical plate theory, and original extensions of it, are derived by using simple concepts from the theory of probability and statistics. Each molecule of a sample chemical substance is examined separately and its motion through the column is described as a stochastic process. Equations for calculating the mean and variance of chromatographic peaks as a function of capacity factor, k, are given for a discrete flow model and a continuous flow model. The variance of position and exit peaks as a function of capacity factor is compared and a simple relationship between the two is derived. The expressions for the mean and variance of chromatographic peaks are used to define plate numbers that describe the separating ability of a chromatographic column under fixed conditions and which, unlike the classical plate numbers N and N_{eff}, are independent of capacity factor, k. In capillary column GC a method is given for determining diffusion coefficients in the gaseous phase that makes it possible to subtract the contribution to peak variance resulting from axial diffusion. When the remaining variance is plotted against $k(1 + k)$, linear regression indicates a straight line with an excellent correlation coefficient and an intercept that is indicative of extra-column peak broadening. A plate number, r', is computed from the slope that is independent of k and can be used to calculate a plate number, r, for any given linear flow-rate. Another simple plotting method gives a plate number that includes the multi-path contribution to peak broadening for packed columns. Numerous examples are given to demonstrate the applicability of these simple concepts to actual chromatographic data.

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CHROMATOGRAPHIC DATA

SUPPLEMENT TO
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TABLE 1181

TABLE OF ISOTACHOPHORETIC INDICES

I. SIMULATED QUALITATIVE AND QUANTITATIVE INDICES OF 287 ANIONIC SUBSTANCES IN THE RANGE pH 3–10

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SUMMARY

A simulation of isotachophoretic equilibria has been applied to 287 anions, evaluating R_E indices for qualitative determination and time-based zone lengths for quantitation under 31 leading electrolyte conditions in the range pH 3–10, using eight different buffers. The R_E values may be useful for correcting asymmetric potentials of sensing electrodes for precise R_E measurement, assessing the separability of samples and estimating the optimum separation conditions. The zone lengths for 10-nmol samples obtained at a driving current of 100 μA may be useful for quantitation.

INTRODUCTION

A unique feature of capillary isotachophoretic apparatus commonly used is that there are no packing materials in the separation column. The isotachophoretic behaviour in such a free electrolyte system can be analyzed theoretically and the observed isotachopherograms can be simulated using a few physico-chemical constants of the sample components and appropriate separation conditions[1,2]. In previous papers we have described applications of this simulative technique to analytical problems such as the assessment of the separability of samples at different pH values[2], estimation of the optimum separation conditions[2] and quantitation without a calibration line[3]. In principle, the separability of samples by isotachophoresis is determined by the effective mobilities of the sample components, which are closely related to their absolute mobilities and pK_a values and to the pH of the leading electrolyte, pH_L, buffered by an appropriate counter ion. To ensure that there is sufficient difference between the effective mobilities of the sample components, a complex-forming technique and a solvent effect are also utilized[4].

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In the present work, the qualitative and quantitative indices of 287 anions are simulated under 31 aqueous electrolyte conditions in the range pH 3–10 by considering the pH dependence of the effective mobility. These indices, *i.e.*, R_E and the time-based zone length, t, can be used as a data base for analytical purposes and for correction of asymmetric potential in the measurement of R_E[5], qualitative identification without addition of a standard and conversion of R_E into other qualitative indices and *vice versa*.

SIMULATION CONDITIONS

The pH of the leading electrolyte, pH_L, was varied in the range 3–10 (0.25 pH units per step) using eight kinds of buffer ions: β-alanine (pH_L = 3–4); ε-aminocaproic acid (4–4.75); creatinine (4.75–5.25); histidine (5.5–6.25); imidazole (6.5–7.25); tris(hydroxymethyl)aminomethane (Tris) (7.5–8.25); 2-amino-2-methyl-1,3-propanediol (amediol) (8.5–9.25); ethanolamine (9.5–10). The absolute mobilities, m_0, and the dissociation constants, pK_a, of the buffers used are summarized in Table I. The absolute mobility of cationic β-alanine ($36.7 \cdot 10^{-5}$ cm^2 V^{-1} sec^{-1}) obtained by conductivity measurement was different from the previously used value[5] of $31.0 \cdot 10^{-5}$ cm^2 V^{-1} sec^{-1} obtained by analysing the step height of anionic β-alanine and assuming the cationic m_0 to be equal to that of the anionic m_0. The leading ion was 0.01 *M* chloride and the driving current was 100 μA. Table II shows the simulation conditions, the simulated concentration of buffer, the effective mobility of the buffer and leading ion, the specific conductivity and the potential gradient of the leading zones. For simulation of the latter the inner diameter of the separation column was assumed to be 0.5 mm. The isotachophoretic zone velocity at each pH_L condition is also shown in Table II. This velocity can be used to estimate the time needed for detecting the first sample zone.

The m_0 and pK_a values of the 287 substances are mainly literature values. For about 80 substances, isotachophoretically evaluated constants were used. It should be noted that the correction of m_0 of β-alanine and revision of the computer program caused little changes in the m_0 and pK_a values evaluated previously[5]. For a part of the samples, especially for isomers of benzene derivatives, pK_a could be found in the

TABLE I

PHYSICO-CHEMICAL CONSTANTS OF BUFFERS USED IN SIMULATION (25°C)

m_0 = Absolute mobility (cm^2 V^{-1} sec^{-1} × 10^5). pK_a = thermodynamic acid dissociation constant. The absolute mobilities were obtained isotachophoretically, and the pK_a values were taken from the literature.

pH_L range	*Buffer*	*pK_a*	*m_0*
3.00–4.00	β-Alanine	3.552	36.7
4.00–4.75	ε-Aminocaproic acid	4.373	28.8
4.75–5.25	Creatinine	4.828	37.2
5.50–6.25	Histidine	6.04	29.6
6.50–7.25	Imidazole	7.15	52.0
7.50–8.25	Tris	8.076	29.5
8.50–9.25	Amediol	8.78	29.5
9.50–10.0	Ethanolamine	9.498	44.3

TABLE II

SIMULATED EFFECTIVE MOBILITIES AND CONCENTRATION OF LEADING ZONE CONSTITUENTS (25°C)

pH_L = pH of leading electrolyte; $\bar{m}_L$ = effective mobility ($cm^2\ V^{-1}\ sec^{-1} \times 10^5$) of leading ion ($Cl^-$), m_0 of Cl^- being $79.08 \cdot 10^{-5}\ cm^2\ V^{-1}\ sec^{-1}$; $C^t_{B,L}$ = total concentration (mM) of buffer ion; $\bar{m}_{B,L}$ = effective mobility ($cm^2\ V^{-1}\ sec^{-1} \times 10^5$) of buffer ion, the counter direction being indicated by a negative sign; κ_L = specific conductivity ($S\ cm^{-1}$) of leading zone; E_L = potential gradient ($V\ cm^{-1}$) of leading zone at a driving current of 100 μA (I.D. of narrow bore tube: 0.5 mm); v = isotachophoretic zone velocity (cm $sec^{-1} \times 10^3$).

Buffer	pH_L	$\bar{m}_L$	$C^t_{B,L}$	$\bar{m}_{B,L}$	κ_L	E_L	v
β-Alanine	3.00	74.64	11.28	−26.48	1.348	37.77	28.20
	3.25	74.61	13.68	−22.88	1.212	41.98	31.32
	3.50	74.57	17.43	−18.43	1.137	44.80	33.40
	3.75	74.51	23.79	−13.70	1.094	46.56	34.69
	4.00	74.44	34.94	−9.40	1.069	47.63	35.46
ε-Aminocaproic acid	4.00	74.60	13.68	−18.41	0.997	51.09	38.12
	4.25	74.58	16.70	−15.15	0.982	51.84	38.65
	4.50	74.48	22.01	−11.52	0.974	52.29	38.94
	4.75	74.40	31.42	−8.08	0.969	52.57	39.11
Creatinine	4.75	74.57	17.50	−19.20	1.050	48.51	36.18
	5.00	74.52	23.37	−14.39	1.047	48.65	36.25
	5.25	74.45	33.80	−9.95	1.045	48.74	36.29
Histidine	5.50	74.63	12.59	−20.82	0.974	52.28	39.02
	5.75	74.59	14.62	−17.93	0.973	52.33	39.03
	6.00	74.53	18.22	−14.39	0.972	52.37	39.03
	6.25	74.46	24.62	−10.65	0.972	52.42	39.03
Imidazole	6.50	74.67	12.02	−40.08	1.202	42.97	32.08
	6.75	74.66	13.59	−35.44	1.185	42.97	32.08
	7.00	74.63	16.38	−29.40	1.185	42.98	32.08
	7.25	74.60	21.35	−22.56	1.185	42.99	32.07
Tris	7.50	74.63	12.39	−21.08	0.972	52.38	39.10
	7.75	74.60	14.26	−18.32	0.972	52.40	39.09
	8.00	74.54	17.57	−14.87	0.971	52.43	39.08
	8.25	74.47	23.46	−11.14	0.971	52.45	39.06
Amediol	8.50	74.59	14.74	−17.73	0.972	52.38	39.07
	8.75	74.53	18.42	−14.19	0.972	52.38	39.04
	9.00	74.45	24.99	−10.46	0.973	52.37	38.99
	9.25	74.37	36.67	−7.14	0.973	52.32	38.91
Ethanolamine	9.50	74.58	19.12	−21.31	1.119	45.53	33.95
	9.75	74.53	26.25	−15.56	1.124	45.32	33.77
	10.00	74.47	39.01	−10.51	1.133	44.94	33.46

literature but m_0 could not. In such cases, the m_0 values were assumed equal to those of compounds of similar structure or similar molecular weight.

The calculations were carried using a SORD microcomputer M223 Mk III

equipped with two 1 MB floppy disk drivers. The results were filed on a floppy disk. To calculate 8897 (287 × 31) R_E values required *ca.* 10 h.

USE OF INDICES

The names of the 287 anionic substances simulated are arranged in alphabetical order in Table III. The simulated results are summarized in Table IV together with values of m_0 and pK_a, the molecular formula and molecular weight. The negative signs of m_0 for anions are omitted except for a few amino acids. Also listed in Table IV are the ratio, R_E, of the potential gradient of the sample zone, E_S, to that of the leading zone, E_L, the time-based zone length, t (sec), the effective charge, $-Z$, and the pH of the sample zone, pH_S, at each pH_L.

I. Correction of asymmetric potential

When a potential gradient detector is used, the actual baseline for the measurement of the step heights of the leading, h_L, and the sample zone, h_S, sometimes drifts due to an asymmetric potential at the sensing electrodes. This drift sometimes results in a significant error in the observed R_E values. In such cases, the simulated R_E values of samples with well defined m_0 and pK_a can be obtained from an evaluation of the drifted step height, Δh. In Table IV, the R_E values of substances marked with (S), R_E (std), are useful as internal standard indices. The Δh can be evaluated as

$$\Delta h = [h_{std} - h_L \cdot R_E(\text{std})]/[R_E(\text{std}) - 1] \quad (1)$$

where h_{std} is the apparent step height of the zone of the internal standard and h_L that of the leading zone. Using Δh, the R_E values of the sample components can be corrected

$$R_E = E_S/E_L = (h_S + \Delta h)/(h_L + \Delta h) \quad (2)$$

where h_S is the observed step height of the sample. Examples of this mode of correction were reported in ref. 5.

II. Assessment of separability

From Table IV, one can assess the separability of the given samples by comparing the R_E indices at the different pH_L values. According to our experience, when the R_E values of two samples coincided within *ca.* 0.15, their separation was difficult or impossible. The linear interpolation of adjacent R_E values gives approximate R_E values at any pH_L using the same buffer: *e.g.*, the R_E values of acetic acid at pH_L 3 and 3.25 are 8.876 and 7.444, then the R_E value at pH_L 3.125 can be estimated as 8.876 − (8.876 − 7.444) × 0.125/0.25 = 8.160. The exactly simulated value is 8.090 and the discrepancy is thus slight.

For the estimation of pH_L and the selection of a terminator for optimum separation, the pH_L should be selected so as to result in sufficient difference between the R_E values of the samples. A plot of R_E against pH_L is useful for this purpose. Fig. 1 shows the dependence on pH_L of the R_E values of benzoate (No. 12 in Table IV), cacodylate (27), caproate (29), chlorate (32), citrate (57), phenolate (229) and N-tris(hydroxymethyl)methyl-3-aminopropanesulphonic acid (TAPS) (262). In the range

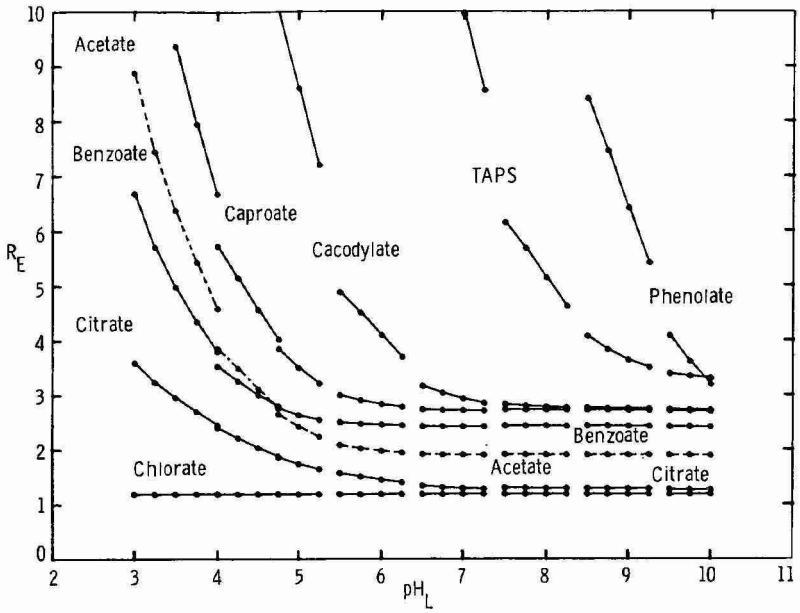

Fig. 1. Effect of pH_L and the buffers on the simulated R_E values of chlorate, citrate, benzoate, acetate, caproate, cacodylate, TAPS and phenolate ions at the isotachophoretically steady state. The leading ion was 10 m*M* Cl^-. The buffers used were β-alanine (pH_L = 3–4), ε-aminocaproic acid (4–4.75), creatinine (4.75–5.25), histidine (5.5–6.25), imidazole (6.5–7.25), tris(hydroxymethyl)aminomethane (7.5–8.25), amediol (8.5–9.25), and ethanolamine (9.5–10).

pH_L 5.5–6.25 histidine buffer, chlorate, citrate, acetate, benzoate and caproate ions can easily be separated using cacodylate ion as terminator. At intermediate pH_L values of 4.5–4.75 (ε-aminocaproic acid buffer), benzoate and acetate ions may form a mixed zone. In the low pH_L range 3–4 the samples can easily be separated, however, cacodylate ion is not suitable as the terminator as the R_E values are too large; caprylate (30) may be suitable. The separability is strongly dependent on the sample amount. For the separation of large amounts of samples, a high loading of leading ion is necessary, even when the difference between R_E values is larger than *ca.* 0.15 (the latter is only a measure of the separation).

III. Qualitative identification

For the identification of unknown samples, the method of standard addition has usually been employed. Instead qualitative identification can be achieved by comparing the observed and simulated R_E values, if the R_E values are measured carefully using an internal standard. At least, the possible candidates for the components in actual samples can be limited to several kinds, and their number can be reduced further by considering the R_E values measured at other pH_L values. This procedure can be performed rapidly by computer-sorting of samples having similar R_E values to those observed.

IV. Quantitation

When the separated samples are identified, their amounts can be determined

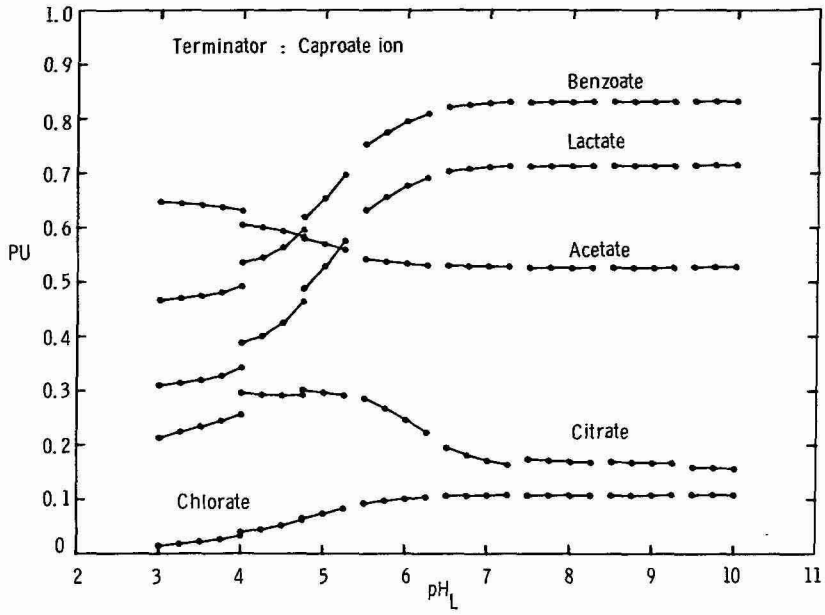

Fig. 2. Effect of pH_L and the buffers on the simulated PU values of chlorate, citrate, lactate, benzoate and acetate ions at the isotachophoretically steady state. The terminator is caproate ion. For the electrolyte systems, see Fig. 1.

using the simulated and observed zone lengths. In Table IV the simulated time-based zone lengths, t(sec), are listed for 10-nmol samples at a driving current of 100 μA. If the observed time-based zone length is t_{obs}(sec) at a driving current of I (μA), the sample amount, n_S(nmol), can be expressed:

$$n_S = t_{obs} I / 10\ t \tag{3}$$

For example, at a driving current of 50 μA and pH_L 6, the time-based zone length of acetic acid was 50 sec. The sample amount can easily be estimated as $50 \times 50/10 \times 16.22 = 15.4$ nmol, and the slope of the calibration line, $I/10t$, is 0.308.

V. Conversion of R_E into different qualitative indices

Besides R_E, several qualitative indices have been proposed such as relative step height[4], IRM[6], PU[7], PR[8], RU (= IRM × 100)[9] and SU (= PU × 100)[9]. The definition of IRM is the same as R_E and PR = $1/R_E$. PU is defined as

$$PU = (h_S - h_L)/(h_T - h_L) \tag{4}$$

where h_T is the step height of the terminating zone. The R_E values of samples can be converted into PU values using the R_E value of the sample, R_E(S), and terminating ion, R_E(T):

$$PU = [R_E(S) - 1]/[R_E(T) - 1] \tag{5}$$

Fig. 2 shows the pH dependence of PU values for acetate (1), benzoate (12), chlorate (32), citrate (57) and lactate (184) using R_E values of caproate ion (29) as the terminator. A similar conversion of the relative step heights of 65 anions[4] to R_E values has been reported in ref. 5.

Thus, the simulated qualitative and quantitative indices can be utilized for several analytical purposes, although the number of simulated samples is limited. It should be noted that the accuracy of the simulated indices depends mainly on the physico-chemical constants of the samples and buffers used. The present table is as yet in an experimental stage, but by continuous revision it will be used widely in future as a data base for isotachophoresis. We await the critical comments of users.

Similar tables for amino acids and cations will be submitted in due course.

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(For Tables III and IV, see pp. D8–D106; references to Table IV are listed on p. D106)

TABLE III

ANIONIC SUBSTANCES LISTED ALPHABETICALLY IN TABLE IV

No.	Samples	No.	Samples
1	ACETIC ACID (S)	49	2-CHLOROPROPIONIC ACID
2	ACRYLIC ACID	50	3-CHLOROPROPIONIC ACID
3	ADIPIC ACID	51	CHLOROUS ACID
4	ALLYLACETIC ACID	52	5-CHLOROVALERIC ACID
5	o-AMINOBENZOIC ACID	53	CHROMIC ACID
6	p-AMINOBENZOIC ACID	54	CINNAMIC ACID
7	ARSENIC ACID	55	cis-CINNAMIC ACID
8	ASPARTIC ACID	56	CITRACONIC ACID
9	ASPIRIN	57	CITRIC ACID (S)
10	AZELAIC ACID	58	CRESOL
11	BENZENESULFONIC ACID	59	m-CRESOL
12	BENZOIC ACID (S)	60	p-CRESOL
13	BENZYLASPARATIC ACID	61	CROTONIC ACID
14	BROMIC ACID (S)	62	CYANIC ACID
15	BROMOACETIC ACID (S)	63	CYANOACETIC ACID
16	m-BROMOBENZOIC ACID	64	m-CYANOBENZOIC ACID
17	o-BROMOBENZOIC ACID	65	CYCLOBUTANE-1,1-DICARBOXYLIC ACID
18	p-BROMOBENZOIC ACID	66	CYCLOHEXANE-1,1-DICARBOXYLIC ACID
19	2-BROMOBUTYRIC ACID	67	CYCLOPENTANE-1,1-DICARBOXYLIC ACID
20	4-BROMOBUTYRIC ACID	68	DECYLSULFONIC ACID
21	o-BROMOPHENYLACETIC ACID	69	DIBROMOFLUOROACETIC ACID
22	2-BROMOPROPIONIC ACID	70	2,3-DIBROMOPROPIONIC ACID
23	5-BROMOVALERIC ACID	71	DICHLOROACETIC ACID (S)
24	o-t-BUTYLBENZOIC ACID	72	DICHLOROFLUOROACETIC ACID
25	p-t-BUTYLBENZOIC ACID	73	2,4-DICHLOROPHENOL
26	BUTYRIC ACID (S)	74	2,4-DICHLOROPHENOXYACETIC ACID
27	CACODYLIC ACID	75	DICHROMIC ACID
28	CAPRIC ACID	76	DIETHYLACETIC ACID
29	CAPROIC ACID (S)	77	DIETHYLMALONIC ACID
30	CAPRYLIC ACID	78	DIFLUOROACETIC ACID
31	CARBONIC ACID	79	2,4-DIHYDROXYBENZOIC ACID
32	CHLORIC ACID (S)	80	2,5-DIHYDROXYBENZOIC ACID
33	2-CHLORO-3-OH-BUTYRIC ACID	81	2,6-DIHYDROXYBENZOIC ACID
34	CHLOROACETIC ACID	82	3,4-DIHYDROXYBENZOIC ACID
35	m-CHLOROBENZOIC ACID	83	3,5-DIHYDROXYBENZOIC ACID
36	o-CHLOROBENZOIC ACID	84	DIHYDROXYTARTARIC ACID
37	p-CHLOROBENZOIC ACID	85	2,3-DIMETHYLBENZOIC ACID
38	2-CHLOROBUTYRIC ACID	86	2,4-DIMETHYLBENZOIC ACID
39	3-CHLOROBUTYRIC ACID	87	2,5-DIMETHYLBENZOIC ACID
40	2-CHLOROCROTONIC ACID	88	2,6-DIMETHYLBENZOIC ACID
41	3-CHLOROCROTONIC ACID	89	3,4-DIMETHYLBENZOIC ACID
42	CHLORODIBROMOACETIC ACID	90	3,5-DIMETHYLBENZOIC ACID
43	CHLORODIFLUOROACETIC ACID	91	DIMETHYLMALONIC ACID
44	2-CHLOROISOCROTONIC ACID	92	2,6-DINITROBENZOIC ACID
45	m-CHLOROPHENOL	93	3,5-DINITROBENZOIC ACID
46	o-CHLOROPHENOL	94	2,3-DINITROPHENOL
47	p-CHLOROPHENOL	95	2,4-DINITROPHENOL
48	p-CHLOROPHENYLACETIC ACID	96	2,5-DINITROPHENOL

No.	Samples	No.	Samples
97	2.6-DINITROPHENOL	145	3-HYDROXY-o-TOLUIC ACID
98	3.4-DINITROPHENOL	146	3-HYDROXY-p-TOLUIC ACID
99	3.5-DINITROPHENOL	147	4-HYDROXY-m-TOLUIC ACID
100	DIPHENYLACETIC ACID	148	6-HYDROXY-o-TOLUIC ACID
101	DIPROPYLMALONIC ACID	149	m-HYDROXYBENZOIC ACID
102	DITHIONIC ACID	150	p-HYDROXYBENZOIC ACID
103	DITHIONOUS ACID	151	2-HYDROXYBUTYRIC ACID
104	DODECYLSULFONIC ACID	152	3-HYDROXYBUTYRIC ACID
105	ENANTHYLIC ACID	153	4-HYDROXYBUTYRIC ACID
106	o-ETHOXYBENZOIC ACID	154	m-HYDROXYCINNAMIC ACID
107	p-ETHOXYBENZOIC ACID	155	o-HYDROXYCINNAMIC ACID
108	o-ETHYLBENZOIC ACID	156	p-HYDROXYCINNAMIC ACID
109	p-ETHYLBENZOIC ACID	157	2-HYDROXYISOBUTYRIC ACID (S)
110	2-ETHYLBUTYRIC ACID	158	p-HYDROXYPHENYLACETIC ACID
111	ETHYLFUMARIC ACID	159	HYDROXYTRIMETHYLACETIC ACID
112	3-ETHYLGLUTARIC ACID	160	2-HYDROXYVALERIC ACID
113	ETHYLMALEIC ACID	161	4-HYDROXYVALERIC ACID
114	ETHYLMALONIC ACID	162	HYPOPHOSPHOROUS ACID (S)
115	ETHYLPROPYLMALONIC ACID	163	IODIC ACID
116	ETHYLSULFONIC ACID	164	IODOACETIC ACID
117	FLUOROACETIC ACID	165	m-IODOBENZOIC ACID
118	m-FLUOROBENZOIC ACID	166	o-IODOBENZOIC ACID
119	o-FLUOROBENZOIC ACID	167	p-IODOBENZOIC ACID
120	p-FLUOROBENZOIC ACID	168	4-IODOBUTYRIC ACID
121	FORMIC ACID (S)	169	m-IODOPHENYLACETIC ACID
122	FUMARIC ACID	170	o-IODOPHENYLACETIC ACID
123	GALLIC ACID	171	p-IODOPHENYLACETIC ACID
124	GLUCONIC ACID	172	3-IODOPROPIONIC ACID
125	GLUCURONIC ACID	173	5-IODOVALERIC ACID
126	GLUTACONIC ACID	174	ISOBUTYRIC ACID
127	GLUTAMIC ACID (S)	175	ISOCAPROIC ACID
128	GLUTARIC ACID	176	ISOCITRIC ACID
129	GLYCERIC ACID	177	ISOPHTHALIC ACID
130	GLYCOLIC ACID	178	o-ISOPROPYLBENZOIC ACID
131	GLYOXYLIC ACID	179	p-ISOPROPYLBENZOIC ACID
132	HIPPURIC ACID	180	ISOPROPYLMALONIC ACID
133	HYDROBROMIC ACID	181	ISOVALERIC ACID
134	HYDROCHLORIC ACID	182	ITACONIC ACID
135	HYDROCYANIC ACID	183	2-KETOGLUTARIC ACID
136	HYDROFLUORIC ACID (S)	184	LACTIC ACID (S)
137	HYDROGEN AZIDE	185	LAURYLSULFONIC ACID
138	HYDROGEN HEXAFLUOROPHOSPHIDE	186	LEVULINIC ACID
139	HYDROGEN SULFIDE	187	MALEIC ACID
140	HYDROIODIC ACID	188	MALIC ACID
141	2-HYDROXY-3-CHLOROBUTYRIC A.	189	MALONIC ACID (S)
142	2-HYDROXY-3-Cl-ISOBUTYRIC A.	190	MANDELIC ACID
143	2-HYDROXY-3-Cl-PROPIONIC A.	191	MES (S)
144	2-HYDROXY-m-TOLUIC ACID	192	MESACONIC ACID

No.	Samples	No.	Samples
193	MESOTARTARIC ACID	241	3-PROPYLGLUTARIC ACID
194	METHACRYLIC ACID	242	PROPYLMALONIC ACID
195	METHOXYACETIC ACID	243	PROPYLSULFONIC ACID
196	m-METHOXYBENZOIC ACID	244	PYRAZOLE-2.3-DICARBOXYLIC ACID
197	o-METHOXYBENZOIC ACID	245	PYROPHOSPHORIC ACID
198	p-METHOXYBENZOIC ACID	246	PYRUVIC ACID
199	p-METHOXYPHENYLACETIC ACID	247	SACCHARIN
200	METHYLETHYLMALONIC ACID	248	SALICYLIC ACID
201	METHYLMALONIC ACID	249	SEBACIC ACID
202	METHYLSULFONIC ACID	250	SELENIC ACID
203	2-NAPHTALENESULFONIC ACID	251	SELENIOUS ACID
204	NICOTINIC ACID	252	SELENOCYANIC ACID
205	NITRIC ACID	253	SORBIC ACID
206	2-NITRO-3-BROMOBENZOIC ACID	254	SUBERIC ACID
207	3-NITRO-2-BROMOBENZOIC ACID	255	SUCCINIC ACID (S)
208	3-NITRO-4-BROMOBENZOIC ACID	256	SULFAMIC ACID (S)
209	2-NITRO-3-CHLOROBENZOIC ACID	257	SULFANILIC ACID
210	3-NITRO-4-CHLOROBENZOIC ACID	258	m-SULFANILIC ACID
211	3-NITRO-5-CHLOROBENZOIC ACID	259	o-SULFANILIC ACID
212	m-NITROBENZOIC ACID	260	SULFURIC ACID
213	o-NITROBENZOIC ACID	261	SULFUROUS ACID
214	p-NITROBENZOIC ACID	262	TAPS
215	m-NITROPHENOL	263	TARTARIC ACID (S)
216	o-NITROPHENOL	264	TARTRONIC ACID
217	p-NITROPHENOL	265	TEREPHTHALIC ACID
218	NITROUS ACID	266	THIOACETIC ACID
219	OCTYLSULFONIC ACID	267	THIOCYANIC ACID
220	OROTIC ACID	268	THIOCYANOACETIC ACID
221	OXALIC ACID (S)	269	THIOGLYCOLIC ACID
222	OXALOACETIC ACID	270	THIOSULFURIC ACID
223	PELARGONIC ACID	271	p-TOLUENESULFONIC ACID
224	PERCHLORIC ACID (S)	272	m-TOLUIC ACID
225	PERIODIC ACID	273	o-TOLUIC ACID
226	PERMANGANIC ACID	274	p-TOLUIC ACID
227	PEROXYSULFURIC ACID	275	TRIBROMOACETIC ACID
228	PERRHENIC ACID	276	TRICHLOROACETIC ACID
229	PHENOL	277	TRICHLOROACRYLIC ACID
230	PHENOXYACETIC ACID	278	TRICHLOROLACTIC ACID
231	PHENYLACETIC ACID	279	TRIMETAPHOSPHORIC ACID
232	4-PHENYLBUTYRIC ACID	280	TRIMETHYLACETIC ACID (S)
233	2-PHENYLPROPIONIC ACID	281	TRIMETHYLACRYLIC ACID
234	3-PHENYLPROPIONIC ACID	282	2.4.6-TRIMETHYLBENZOIC ACID
235	PHOSPHORIC ACID (S)	283	TRIMETYLPYRUVIC ACID
236	PHOSPHOROUS ACID	284	VALERIC ACID
237	PHTHALIC ACID	285	VANILLIC ACID
238	PICRIC ACID	286	VINYLACETIC ACID
239	PIMELIC ACID	287	VINYLGLYCOLIC ACID
240	PROPIONIC ACID (S)		

TABLE IV

ISOTACHOPHORETIC INDICES OF 287 ANIONIC SUBSTANCES

1 ACETIC ACID (S) C2H4O2

-1	42.4	4.756	60.05				pHL	3.00	3.25	3.50
							RE	8.876	7.444	6.370
							t	21.01	20.13	19.51
							Z	0.206	0.247	0.289
							pHS	4.151	4.249	4.342

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.428	4.576	3.848	3.485	3.111	2.763	2.650	2.427	2.244	2.087	2.027
19.02	18.64	16.48	16.37	16.26	16.18	18.16	18.12	18.09	16.23	16.22
0.340	0.404	0.485	0.537	0.603	0.681	0.711	0.778	0.843	0.912	0.940
4.443	4.561	4.700	4.789	4.904	5.050	5.112	5.264	5.449	5.733	5.910
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.980	1.949	1.925	1.915	1.909	1.904	1.912	1.910	1.909	1.908	1.909
16.22	16.21	21.62	21.61	21.61	21.61	16.18	16.18	16.19	16.20	16.20
0.962	0.978	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.122	6.355	6.651	6.887	7.132	7.380	7.593	7.841	8.091	8.340	8.591
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1				
1.908	1.907	1.906	1.902	1.901	1.899					
16.23	16.27	16.34	20.09	20.36	20.85					
1.000	1.000	1.000	1.000	1.000	1.000					
8.842	9.092	9.343	9.626	9.878	10.133					

2 ACRYLIC ACID C3H4O2

-1	42.7	4.258	72.06				pHL	3.00	3.25	3.50
							RE	5.663	4.816	4.183
							t	21.28	20.26	19.56
							Z	0.324	0.382	0.441
							pHS	3.914	4.023	4.127

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.635	3.153	2.863	2.638	2.422	2.241	2.206	2.093	2.012	1.963	1.936
19.00	18.59	16.48	16.34	16.21	16.12	18.11	18.06	18.03	16.18	16.17
0.509	0.588	0.653	0.710	0.775	0.839	0.853	0.900	0.937	0.964	0.978
4.244	4.382	4.498	4.611	4.758	4.938	4.983	5.173	5.390	5.650	5.865
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.918	1.907	1.896	1.893	1.890	1.888	1.896	1.896	1.895	1.893	1.895
16.16	16.16	21.53	21.53	21.52	21.52	16.13	16.13	16.14	16.15	16.15
0.987	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.100	6.344	6.634	6.879	7.128	7.377	7.590	7.839	8.089	8.339	8.590
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 3				
1.894	1.893	1.892	1.889	1.887	1.885					
16.18	16.22	16.29	20.01	20.27	20.76					
1.000	1.000	1.000	1.000	1.000	1.000					
8.840	9.091	9.341	9.624	9.877	10.131					

3 ADIPIC ACID C6H10O4

-1	24.6	4.430	146.14				pHL	3.00	3.25	3.50
-2	52.4	5.277					RE	9.612	7.981	6.740
							t	31.81	30.07	29.04
							Z	0.335	0.404	0.480
							pHS	4.042	4.147	4.248

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.657	4.689	4.086	3.601	3.124	2.698	2.587	2.307	2.086	1.918	1.840
28.45	28.28	25.15	25.48	26.02	26.77	30.54	31.29	32.03	29.61	29.95
0.574	0.695	0.807	0.919	1.062	1.234	1.286	1.446	1.602	1.764	1.840
4.359	4.489	4.599	4.705	4.839	5.002	5.055	5.223	5.419	5.692	5.882
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.783	1.745	1.708	1.696	1.687	1.680	1.703	1.701	1.698	1.696	1.699
30.22	30.39	40.01	40.06	40.07	40.06	30.61	30.62	30.62	30.63	30.66
1.900	1.941	1.968	1.982	1.990	1.994	1.996	1.998	1.999	1.999	2.000
6.102	6.338	6.625	6.863	7.108	7.356	7.577	7.826	8.076	8.325	8.576
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.697	1.695	1.693	1.682	1.678	1.675					
30.69	30.75	30.85	37.38	37.77	38.49					
2.000	2.000	2.000	2.000	2.000	2.000					
8.826	9.076	9.327	9.603	9.854	10.107					

4 ALLYLACETIC ACID C5H8O2

-1	33.9	4.674	100.12				pHL	3.00	3.25	3.50
							RE	10.017	8.409	7.202
							t	24.29	23.04	22.18
							Z	0.230	0.275	0.322
							pHS	4.130	4.232	4.328

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.150	5.208	4.527	4.100	3.673	3.288	3.176	2.930	2.736	2.595	2.530
21.51	21.01	18.32	18.17	18.03	17.93	20.44	20.39	20.35	18.01	18.00
0.378	0.448	0.521	0.576	0.645	0.723	0.749	0.814	0.873	0.928	0.952
4.434	4.558	4.681	4.777	4.902	5.058	5.116	5.281	5.477	5.745	5.936
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.483	2.451	2.423	2.413	2.407	2.402	2.418	2.416	2.414	2.412	2.415
17.99	17.99	24.82	24.82	24.81	24.81	17.95	17.96	17.96	17.97	17.99
0.971	0.983	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.157	6.394	6.702	6.942	7.188	7.437	7.635	7.884	8.134	8.384	8.636
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 3				
2.413	2.411	2.408	2.402	2.398	2.394					
18.03	18.09	18.19	23.02	23.47	24.34					
1.000	1.000	1.000	1.000	1.000	1.000					
8.886	9.137	9.388	9.686	9.941	10.199					

5 o-AMINOBENZOIC ACID C7H7NO2

1	31.6	2.108	137.10				pHL	3.00	3.25	3.50
-1	-31.6	4.939					RE	13.704	11.444	9.740
							t	25.78	24.32	23.32
							Z	0.180	0.216	0.254
							pHS	4.282	4.374	4.462

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
8.245	6.895	5.799	5.208	4.602	4.038	3.835	3.472	3.169	2.909	2.808
22.54	21.95	19.01	18.84	18.70	18.58	21.27	21.22	21.18	18.67	18.66
0.301	0.362	0.435	0.485	0.551	0.631	0.665	0.736	0.809	0.890	0.923
4.559	4.674	4.802	4.888	5.000	5.141	5.206	5.353	5.533	5.810	5.980
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.727	2.672	2.623	2.606	2.595	2.588	2.607	2.603	2.601	2.598	2.601
18.65	18.65	26.00	25.99	25.99	25.98	18.61	18.61	18.62	18.63	18.65
0.951	0.970	0.985	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000
6.188	6.417	6.730	6.965	7.209	7.457	7.652	7.900	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
2.599	2.596	2.593	2.585	2.581	2.576					
18.69	18.76	18.88	24.12	24.66	25.72					
1.000	1.000	1.000	1.000	1.000	1.000					
8.901	9.152	9.404	9.707	9.963	10.223					

6 p-AMINOBENZOIC ACID C7H7NO2

1	31.6	2.413	137.10				pHL	3.00	3.25	3.50
-1	-31.6	4.853					RE	12.621	10.570	9.018
							t	26.28	24.68	23.57
							Z	0.196	0.234	0.275
							pHS	4.259	4.346	4.432

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.653	6.422	5.459	4.915	4.361	3.849	3.678	3.349	3.081	2.865	2.775
22.70	22.05	19.07	18.88	18.72	18.59	21.28	21.22	21.18	18.67	18.66
0.325	0.389	0.463	0.515	0.583	0.663	0.694	0.764	0.833	0.904	0.934
4.528	4.643	4.767	4.856	4.972	5.117	5.179	5.333	5.518	5.791	5.969
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.706	2.659	2.617	2.603	2.593	2.587	2.606	2.603	2.600	2.598	2.601
18.65	18.65	26.00	25.99	25.99	25.98	18.61	18.61	18.62	18.63	18.65
0.959	0.975	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.181	6.414	6.727	6.963	7.209	7.457	7.651	7.900	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
2.599	2.596	2.593	2.585	2.581	2.576					
18.69	18.76	18.88	24.12	24.66	25.72					
1.000	1.000	1.000	1.000	1.000	1.000					
8.901	9.152	9.404	9.707	9.963	10.223					

7 ARSENIC ACID H3AsO4 141.94

-1	35.2	2.190					pHL	3.00	3.25	3.50
-2	70.0	6.940					RE	2.463	2.407	2.370
							t	27.10	24.32	22.57
							Z	0.936	0.959	0.974
							pHS	3.318	3.513	3.713

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.344	2.326	2.336	2.324	2.312	2.297	2.293	2.272	2.238	2.186	2.104
21.43	20.74	18.38	18.03	17.85	17.81	20.28	20.38	20.62	18.92	19.64
0.985	0.992	0.993	0.998	1.003	1.009	1.010	1.020	1.036	1.069	1.114
3.930	4.162	4.171	4.396	4.634	4.879	4.905	5.152	5.400	5.690	5.928
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.993	1.857	1.619	1.527	1.440	1.367	1.321	1.291	1.270	1.257	1.251
20.64	21.86	30.76	31.62	32.45	33.13	26.77	27.04	27.24	27.36	27.44
1.182	1.277	1.479	1.577	1.682	1.779	1.866	1.914	1.948	1.970	1.983
6.162	6.392	6.768	6.935	7.127	7.340	7.598	7.811	8.044	8.287	8.537
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 4				
1.246	1.243	1.241	1.234	1.232	1.231					
27.50	27.56	27.64	32.36	32.58	32.97					
1.990	1.994	1.997	1.998	1.999	1.999					
8.784	9.032	9.282	9.541	9.792	10.042					

8 ASPARTIC ACID C4H7NO4 133.10

1	31.6	1.990					pHL	3.00	3.25	3.50
-1	-31.6	3.900					RE	5.614	4.865	4.305
-2	-51.8	10.002					t	26.69	24.86	23.61
							Z	0.449	0.520	0.589
							pHS	3.807	3.922	4.038

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.832	3.437	3.311	3.107	2.932	2.801	2.781	2.703	2.653	2.640	2.623
22.67	22.00	19.19	18.92	18.71	18.57	21.32	21.24	21.20	18.68	18.66
0.664	0.743	0.777	0.830	0.881	0.923	0.929	0.956	0.974	0.985	0.991
4.173	4.334	4.412	4.555	4.734	4.943	4.982	5.201	5.436	5.674	5.909
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.611	2.603	2.589	2.585	2.581	2.576	2.594	2.587	2.574	2.553	2.523
18.65	18.65	26.02	26.02	26.04	26.06	18.72	18.81	18.96	19.23	19.71
0.995	0.997	0.999	1.000	1.002	1.003	1.006	1.010	1.018	1.032	1.057
6.153	6.400	6.709	6.957	7.206	7.456	7.653	7.903	8.153	8.403	8.669
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.470	2.391	2.287	2.131	2.014	1.911					
20.45	21.57	23.09	31.05	33.26	35.62					
1.098	1.161	1.253	1.400	1.531	1.661					
8.917	9.162	9.405	9.699	9.925	10.157					

9 ASPIRIN C9H8O4 180.16

-1	26.7	3.485					pHL	3.00	3.25	3.50
							RE	4.917	4.415	4.042
							t	30.70	28.20	26.51
							Z	0.617	0.689	0.755
							pHS	3.663	3.800	3.942

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.740	3.506	3.488	3.359	3.260	3.193	3.180	3.142	3.117	3.127	3.119
25.29	24.45	21.20	20.81	20.53	20.36	23.65	23.55	23.49	20.49	20.47
0.818	0.875	0.886	0.921	0.950	0.970	0.972	0.984	0.991	0.994	0.997
4.105	4.296	4.340	4.517	4.725	4.954	4.991	5.226	5.470	5.698	5.941
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.112	3.106	3.088	3.086	3.083	3.079	3.112	3.110	3.107	3.104	3.109
20.46	20.45	29.23	29.22	29.21	29.20	20.41	20.42	20.42	20.44	20.47
0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.189	6.438	6.755	7.005	7.254	7.504	7.688	7.937	8.187	8.438	8.690
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 3				
3.106	3.102	3.098	3.084	3.078	3.069					
20.53	20.62	20.80	27.20	28.05	29.79					
1.000	1.000	1.000	1.000	1.000	1.000					
8.941	9.192	9.444	9.762	10.020	10.287					

10 AZELAIC ACID C9H1604 188.22

-1	22.0	4.550					pHL	3.00	3.25	3.50
-2	45.9	5.333					RE	11.739	9.723	8.186
							t	34.49	32.49	31.28
							Z	0.307	0.373	0.444
							pHS	4.110	4.213	4.311

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.845	5.647	4.905	4.307	3.719	3.195	3.048	2.705	2.434	2.233	2.138
30.56	30.31	26.70	27.00	27.52	28.26	32.55	33.33	34.13	31.30	31.69
0.534	0.651	0.761	0.871	1.014	1.189	1.245	1.410	1.575	1.745	1.827
4.420	4.546	4.652	4.754	4.883	5.041	5.096	5.260	5.452	5.720	5.908
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.067	2.020	1.973	1.958	1.947	1.939	1.971	1.968	1.964	1.961	1.965
31.98	32.18	43.29	43.33	43.35	43.34	32.44	32.44	32.45	32.46	32.50
1.892	1.936	1.966	1.980	1.989	1.994	1.996	1.998	1.999	1.999	2.000
6.127	6.362	6.657	6.896	7.141	7.389	7.602	7.850	8.100	8.349	8.601
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.963	1.960	1.956	1.941	1.936	1.931					
32.54	32.61	32.74	40.34	40.86	41.85					
2.000	2.000	2.000	2.000	2.000	2.000					
8.851	9.101	9.352	9.636	9.888	10.142					

11 BENZENESULFONIC ACID C6H603S 158.17

-1	38.7	-2.000					pHL	3.00	3.25	3.50
							RE	2.093	2.093	2.093
							t	25.93	23.10	21.37
							Z	1.000	1.000	1.000
							pHS	3.239	3.453	3.669

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.092	2.092	2.100	2.100	2.099	2.097	2.096	2.094	2.093	2.101	2.101
20.29	19.64	17.51	17.16	16.95	16.83	19.05	18.99	18.95	16.90	16.89
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.896	4.134	4.137	4.369	4.611	4.857	4.878	5.126	5.375	5.609	5.858
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.100	2.098	2.093	2.092	2.091	2.090	2.102	2.101	2.100	2.098	2.101
16.89	16.88	22.83	22.83	22.83	22.82	16.85	16.85	16.86	16.87	16.88
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.107	6.357	6.651	6.901	7.151	7.401	7.607	7.857	8.107	8.357	8.608
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
2.099	2.098	2.096	2.092	2.090	2.087					
16.91	16.95	17.04	21.19	21.52	22.14					
1.000	1.000	1.000	1.000	1.000	1.000					
8.859	9.109	9.360	9.650	9.903	10.159					

12 BENZOIC ACID C7H602 122.12

-1	33.6	4.203					pHL	3.00	3.25	3.50
							RE	6.683	5.705	4.971
							t	24.91	23.46	22.47
							Z	0.352	0.413	0.476
							pHS	3.913	4.025	4.134

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.339	3.791	3.525	3.255	3.004	2.801	2.762	2.637	2.551	2.509	2.480
21.72	21.16	18.49	18.29	18.12	18.00	20.56	20.50	20.46	18.09	18.08
0.547	0.628	0.681	0.739	0.803	0.863	0.875	0.917	0.949	0.971	0.982
4.256	4.400	4.500	4.622	4.778	4.967	5.012	5.212	5.435	5.683	5.905
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.460	2.448	2.432	2.428	2.425	2.422	2.440	2.438	2.436	2.434	2.437
18.07	18.07	24.97	24.96	24.96	24.95	18.03	18.04	18.04	18.06	18.07
0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.144	6.389	6.694	6.940	7.189	7.438	7.636	7.886	8.136	8.386	8.637
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.436	2.433	2.431	2.424	2.421	2.417					
18.11	18.17	18.28	23.16	23.62	24.51					
1.000	1.000	1.000	1.000	1.000	1.000					
8.888	9.138	9.390	9.689	9.944	10.202					

13 BENZYLASPARATIC ACID C11H13NO4 223.23

1	25.8	-3.000								
-1	-25.8	4.855								

pHL	3.00	3.25	3.50
RE	14.983	12.525	10.669
t	29.33	27.56	26.35
Z	0.203	0.243	0.287
pHS	4.243	4.344	4.439

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
9.051	7.605	6.621	5.944	5.269	4.659	4.463	4.070	3.758	3.531	3.423
25.44	24.77	21.23	21.03	20.86	20.73	24.07	24.01	23.98	20.89	20.87
0.339	0.406	0.471	0.527	0.597	0.678	0.708	0.778	0.845	0.909	0.939
4.544	4.666	4.779	4.874	4.996	5.147	5.209	5.369	5.560	5.822	6.007

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.342	3.288	3.233	3.217	3.206	3.198	3.231	3.227	3.224	3.219	3.225
20.86	20.86	29.96	29.95	29.94	29.93	20.82	20.83	20.84	20.85	20.89
0.962	0.978	0.989	0.994	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.224	6.459	6.782	7.021	7.267	7.515	7.698	7.946	8.196	8.446	8.699

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10
3.221	3.217	3.212	3.197	3.190	3.180	
20.95	21.05	21.24	27.92	28.85	30.80	
1.000	1.000	1.000	1.000	1.000	1.000	
8.950	9.201	9.453	9.774	10.033	10.301	

14 BROMIC ACID (S) HBrO3 128.91

-1	57.8	-2.000								

pHL	3.00	3.25	3.50
RE	1.381	1.381	1.381
t	20.82	18.65	17.38
Z	1.000	1.000	1.000
pHS	3.101	3.333	3.567

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.380	1.380	1.382	1.382	1.382	1.381	1.381	1.381	1.380	1.383	1.382
16.62	16.19	14.80	14.55	14.41	14.34	15.80	15.76	15.73	14.38	14.37
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.806	4.051	4.053	4.295	4.542	4.790	4.799	5.048	5.298	5.541	5.790

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.382	1.382	1.381	1.380	1.380	1.380	1.383	1.382	1.382	1.382	1.382
14.37	14.37	18.28	18.28	18.29	18.29	14.34	14.35	14.35	14.36	14.36
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.040	6.290	6.559	6.809	7.059	7.309	7.540	7.790	8.040	8.290	8.540

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 12
1.382	1.382	1.381	1.380	1.380	1.379	
14.38	14.40	14.44	17.11	17.25	17.51	
1.000	1.000	1.000	1.000	1.000	1.000	
8.791	9.041	9.291	9.556	9.807	10.059	

15 BROMOACETIC ACID (S) C2H3BrO2 138.95

-1	40.6	2.901								

pHL	3.00	3.25	3.50
RE	2.556	2.374	2.247
t	23.93	21.93	20.62
Z	0.773	0.834	0.882
pHS	3.398	3.565	3.738

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.154	2.089	2.090	2.054	2.030	2.014	2.012	2.003	1.997	2.002	2.000
19.72	19.13	17.07	16.77	16.58	16.47	18.58	18.52	18.49	16.54	16.53
0.922	0.951	0.954	0.971	0.983	0.990	0.990	0.995	0.997	0.998	0.999
3.933	4.150	4.176	4.384	4.613	4.854	4.876	5.119	5.366	5.603	5.850

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.998	1.996	1.991	1.990	1.989	1.988	1.999	1.998	1.997	1.996	1.998
16.52	16.52	22.18	22.18	22.17	22.17	16.49	16.49	16.50	16.51	16.52
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.099	6.348	6.639	6.889	7.139	7.389	7.598	7.848	8.098	8.348	8.599

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1
1.997	1.995	1.994	1.990	1.988	1.986	
16.54	16.58	16.66	20.60	20.89	21.44	
1.000	1.000	1.000	1.000	1.000	1.000	
8.850	9.100	9.351	9.637	9.890	10.145	

16 m-BROMOBENZOIC ACID C7H5BrO2

-1	31.5	3.812	201.02				pHL	3.00	3.25	3.50
							RE	5.249	4.582	4.082
							t	26.63	24.82	23.59
							Z	0.483	0.555	0.625
							pHS	3.755	3.879	4.003
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.662	3.316	3.222	3.040	2.886	2.775	2.758	2.692	2.650	2.642	2.628
22.67	22.02	19.22	18.95	18.74	18.60	21.36	21.28	21.23	18.71	18.69
0.698	0.774	0.802	0.852	0.898	0.936	0.940	0.964	0.979	0.987	0.993
4.145	4.314	4.385	4.536	4.722	4.936	4.974	5.197	5.434	5.671	5.908
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.618	2.611	2.598	2.595	2.593	2.590	2.611	2.610	2.608	2.606	2.609
18.68	18.68	26.06	26.05	26.05	26.04	18.64	18.64	18.65	18.66	18.68
0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.153	6.401	6.709	6.957	7.206	7.456	7.650	7.899	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.607	2.605	2.602	2.593	2.589	2.584					
18.72	18.79	18.92	24.17	24.72	25.78					
1.000	1.000	1.000	1.000	1.000	1.000					
8.902	9.153	9.404	9.708	9.964	10.224					

17 o-BROMOBENZOIC ACID C7H5BrO2

-1	31.5	2.854	201.02				pHL	3.00	3.25	3.50
							RE	3.183	2.993	2.860
							t	28.37	25.76	24.03
							Z	0.810	0.862	0.904
							pHS	3.449	3.617	3.791
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.763	2.695	2.705	2.667	2.641	2.624	2.619	2.609	2.602	2.614	2.611
22.85	22.08	19.40	19.01	18.75	18.60	21.37	21.29	21.24	18.71	18.69
0.936	0.961	0.962	0.976	0.986	0.992	0.992	0.996	0.998	0.999	0.999
3.987	4.205	4.225	4.434	4.663	4.904	4.933	5.177	5.424	5.654	5.901
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.609	2.606	2.595	2.594	2.592	2.590	2.611	2.610	2.608	2.605	2.609
18.68	18.68	26.06	26.05	26.05	26.04	18.64	18.64	18.65	18.66	18.68
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.150	6.399	6.707	6.956	7.206	7.456	7.649	7.899	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.607	2.605	2.602	2.593	2.589	2.584					
18.72	18.79	18.92	24.17	24.72	25.78					
1.000	1.000	1.000	1.000	1.000	1.000					
8.902	9.153	9.404	9.708	9.964	10.224					

18 p-BROMOBENZOIC ACID C7H5BrO2

-1	31.5	3.971	201.02				pHL	3.00	3.25	3.50
							RE	5.890	5.093	4.493
							t	26.38	24.67	23.51
							Z	0.429	0.497	0.566
							pHS	3.821	3.939	4.057
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.985	3.555	3.406	3.184	2.990	2.843	2.819	2.731	2.673	2.655	2.635
22.63	22.00	19.18	18.93	18.74	18.60	21.35	21.28	21.23	18.71	18.69
0.640	0.720	0.757	0.812	0.866	0.912	0.919	0.949	0.970	0.982	0.990
4.190	4.349	4.431	4.571	4.745	4.950	4.991	5.206	5.439	5.679	5.911
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.622	2.614	2.599	2.596	2.593	2.590	2.611	2.610	2.608	2.606	2.609
18.68	18.68	26.06	26.05	26.05	26.04	18.64	18.64	18.65	18.66	18.68
0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.154	6.401	6.709	6.957	7.207	7.456	7.650	7.899	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.607	2.605	2.602	2.593	2.589	2.584					
18.72	18.79	18.92	24.17	24.72	25.78					
1.000	1.000	1.000	1.000	1.000	1.000					
8.902	9.153	9.404	9.708	9.964	10.224					

19 2-BROMOBUTYRIC ACID C4H7BrO2

-1	32.3	2.987			167.00		pHL	3.00	3.25	3.50
							RE	3.263	3.033	2.870
							t	27.66	25.22	23.61
							Z	0.768	0.828	0.876
							pHS	3.474	3.635	3.803

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.747	2.661	2.667	2.618	2.585	2.563	2.558	2.545	2.537	2.547	2.544
22.48	21.75	19.12	18.75	18.51	18.36	21.06	20.98	20.93	18.46	18.45
0.917	0.947	0.950	0.968	0.981	0.989	0.990	0.994	0.997	0.998	0.999
3.992	4.206	4.231	4.435	4.661	4.900	4.929	5.171	5.418	5.649	5.896

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.541	2.538	2.528	2.527	2.525	2.522	2.543	2.541	2.540	2.537	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.144	6.394	6.700	6.949	7.199	7.449	7.644	7.894	8.144	8.394	8.646

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.539	2.537	2.534	2.526	2.523	2.518	
18.48	18.54	18.66	23.77	24.28	25.27	
1.000	1.000	1.000	1.000	1.000	1.000	
8.896	9.147	9.399	9.701	9.956	10.215	

20 4-BROMOBUTYRIC ACID C4H7BrO2

-1	34.4	4.585			167.00		pHL	3.00	3.25	3.50
							RE	9.113	7.670	6.586
							t	24.13	22.87	22.01
							Z	0.250	0.297	0.347
							pHS	4.086	4.190	4.288

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.643	4.802	4.224	3.839	3.456	3.116	3.025	2.809	2.643	2.529	2.473
21.34	20.84	18.20	18.04	17.90	17.80	20.28	20.22	20.19	17.88	17.87
0.407	0.480	0.551	0.607	0.677	0.753	0.776	0.837	0.891	0.938	0.960
4.396	4.523	4.643	4.743	4.873	5.034	5.090	5.261	5.463	5.728	5.925

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.433	2.407	2.383	2.375	2.369	2.365	2.381	2.379	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.976	0.986	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.150	6.389	6.695	6.937	7.184	7.433	7.632	7.881	8.131	8.381	8.632

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.376	2.374	2.372	2.365	2.362	2.358	
17.89	17.95	18.06	22.80	23.24	24.08	
1.000	1.000	1.000	1.000	1.000	1.000	
8.883	9.133	9.385	9.682	9.936	10.195	

21 o-BROMOPHENYLACETIC ACID C8H7BrO2

-1	31.4	4.054			215.05		pHL	3.00	3.25	3.50
							RE	6.292	5.416	4.757
							t	26.31	24.65	23.51
							Z	0.402	0.468	0.535
							pHS	3.857	3.973	4.087

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.195	3.715	3.529	3.284	3.067	2.897	2.868	2.766	2.698	2.673	2.650
22.65	22.04	19.20	18.96	18.77	18.63	21.39	21.32	21.27	18.74	18.72
0.609	0.690	0.732	0.788	0.846	0.897	0.906	0.940	0.964	0.979	0.988
4.217	4.370	4.457	4.591	4.760	4.960	5.002	5.213	5.443	5.684	5.914

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.634	2.624	2.609	2.605	2.602	2.599	2.620	2.619	2.617	2.614	2.618
18.71	18.71	26.11	26.11	26.10	26.09	18.67	18.67	18.68	18.69	18.72
0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.156	6.402	6.711	6.959	7.208	7.457	7.650	7.900	8.150	8.400	8.652

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2
2.616	2.613	2.610	2.602	2.598	2.593	
18.75	18.82	18.95	24.23	24.78	25.85	
1.000	1.000	1.000	1.000	1.000	1.000	
8.903	9.153	9.405	9.709	9.965	10.225	

22 2-BROMOPROPIONIC ACID C3H5BrO2
-1 33.4 2.975 152.98

pHL	3.00	3.25	3.50
RE	3.149	2.927	2.769
t	27.05	24.69	23.12
Z	0.768	0.828	0.877
pHS	3.463	3.625	3.793

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.651	2.568	2.573	2.527	2.495	2.474	2.470	2.457	2.449	2.459	2.455
22.03	21.32	18.79	18.43	18.20	18.06	20.66	20.58	20.53	18.15	18.14
0.917	0.948	0.951	0.969	0.981	0.989	0.990	0.994	0.997	0.998	0.999
3.983	4.197	4.223	4.427	4.654	4.893	4.921	5.163	5.410	5.642	5.888
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.453	2.450	2.441	2.440	2.438	2.436	2.454	2.453	2.451	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.137	6.387	6.691	6.940	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

23 5-BROMOVALERIC ACID C5H9BrO2
-1 32.3 4.721 181.03

pHL	3.00	3.25	3.50
RE	10.913	9.150	7.825
t	25.06	23.74	22.83
Z	0.222	0.265	0.311
pHS	4.157	4.258	4.354

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.670	5.635	4.888	4.418	3.947	3.521	3.393	3.120	2.905	2.745	2.673
22.12	21.60	18.77	18.61	18.47	18.36	21.01	20.95	20.92	18.46	18.45
0.366	0.435	0.507	0.562	0.631	0.710	0.737	0.804	0.865	0.923	0.949
4.459	4.582	4.704	4.800	4.923	5.077	5.136	5.299	5.493	5.761	5.949
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.618	2.583	2.550	2.539	2.532	2.526	2.545	2.543	2.540	2.538	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.968	0.981	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.169	6.405	6.716	6.955	7.202	7.450	7.646	7.895	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

24 o-t-BUTYLBENZOIC ACID C11H14O2
-1 23.2 3.535 178.23

pHL	3.00	3.25	3.50
RE	5.717	5.137	4.704
t	34.09	31.20	29.25
Z	0.614	0.685	0.751
pHS	3.709	3.845	3.985

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.352	4.076	4.062	3.909	3.791	3.711	3.693	3.647	3.617	3.634	3.623
27.83	26.87	23.10	22.65	22.33	22.13	25.94	25.83	25.76	22.29	22.26
0.814	0.872	0.883	0.919	0.948	0.969	0.971	0.983	0.990	0.994	0.997
4.147	4.336	4.378	4.554	4.761	4.990	5.030	5.265	5.509	5.733	5.976
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.615	3.607	3.581	3.578	3.574	3.570	3.615	3.612	3.609	3.604	3.611
22.25	22.24	32.42	32.41	32.39	32.38	22.20	22.21	22.22	22.24	22.28
0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.224	6.473	6.799	7.048	7.298	7.547	7.723	7.973	8.223	8.473	8.727
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.607	3.602	3.596	3.575	3.565	3.551					
22.36	22.49	22.73	30.36	31.65	34.47					
1.000	1.000	1.000	1.000	1.000	1.000					
8.978	9.229	9.482	9.813	10.075	10.350					

25 p-t-BUTYLBENZOIC ACID C11H14O2

-1	23.2	4.400	178.23				pHL	3.00	3.25	3.50
							RE	10.773	9.164	7.940
							t	32.41	30.15	28.63
							Z	0.318	0.376	0.435
							pHS	4.049	4.158	4.264

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.882	5.958	5.554	5.080	4.640	4.278	4.193	3.969	3.813	3.746	3.691
27.50	26.69	22.80	22.51	22.27	22.10	25.88	25.80	25.74	22.28	22.26
0.505	0.586	0.636	0.697	0.766	0.834	0.849	0.899	0.937	0.963	0.977
4.383	4.524	4.613	4.732	4.884	5.067	5.120	5.317	5.537	5.775	5.995
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.654	3.630	3.592	3.584	3.577	3.572	3.616	3.613	3.609	3.605	3.611
22.25	22.24	32.42	32.40	32.39	32.38	22.20	22.21	22.22	22.24	22.28
0.987	0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.232	6.477	6.804	7.050	7.298	7.548	7.723	7.973	8.223	8.473	8.727
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.607	3.602	3.596	3.575	3.565	3.551					
22.36	22.49	22.73	30.36	31.65	34.47					
1.000	1.000	1.000	1.000	1.000	1.000					
8.978	9.229	9.482	9.813	10.075	10.350					

26 BUTYRIC ACID (S) C4H8O2

-1	33.8	4.820	88.11				pHL	3.00	3.25	3.50
							RE	11.526	9.640	8.224
							t	24.23	23.01	22.18
							Z	0.200	0.240	0.282
							pHS	4.200	4.299	4.392

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.987	5.874	4.999	4.507	4.007	3.546	3.394	3.097	2.856	2.659	2.578
21.53	21.03	18.33	18.18	18.06	17.95	20.47	20.42	20.38	18.04	18.03
0.333	0.397	0.471	0.524	0.592	0.671	0.702	0.771	0.838	0.908	0.937
4.495	4.614	4.743	4.833	4.950	5.097	5.159	5.313	5.499	5.775	5.953
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.516	2.474	2.438	2.425	2.417	2.411	2.427	2.424	2.422	2.420	2.422
18.02	18.02	24.87	24.86	24.86	24.85	17.98	17.98	17.99	18.00	18.02
0.960	0.976	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.166	6.399	6.708	6.945	7.190	7.438	7.637	7.885	8.135	8.384	8.636
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.421	2.418	2.416	2.409	2.406	2.402					
18.05	18.11	18.22	23.07	23.52	24.40					
1.000	1.000	1.000	1.000	1.000	1.000					
8.887	9.137	9.388	9.687	9.942	10.200					

27 CACODYLIC ACID (S) C2H7AsO2

-1	29.9	6.184	138.00				pHL	3.00	3.25	3.50
							RE	53.330	43.793	36.666
							t	25.77	24.52	23.67
							Z	0.048	0.058	0.070
							pHS	4.877	4.967	5.049

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
30.417	24.720	18.467	16.251	13.887	11.544	10.054	8.598	7.202	4.876	4.509
23.00	22.48	19.41	19.30	19.19	19.10	21.87	21.84	21.81	19.21	19.21
0.084	0.104	0.141	0.160	0.188	0.226	0.261	0.306	0.367	0.552	0.598
5.137	5.236	5.382	5.447	5.530	5.631	5.712	5.807	5.924	6.246	6.327
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
4.097	3.701	3.170	3.042	2.932	2.851	2.832	2.801	2.781	2.767	2.765
19.20	19.20	26.95	26.95	26.96	26.96	19.16	19.17	19.17	19.19	19.21
0.661	0.734	0.859	0.896	0.931	0.957	0.973	0.984	0.991	0.995	0.997
6.442	6.591	6.934	7.085	7.278	7.498	7.704	7.929	8.169	8.414	8.666
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
2.759	2.754	2.750	2.739	2.735	2.728					
19.25	19.33	19.47	25.06	25.68	26.92					
0.998	0.999	0.999	1.000	1.000	1.000					
8.915	9.165	9.417	9.725	9.981	10.243					

28 CAPRIC ACID C10H2002

-1	22.1	5.000	172.27							

pHL	3.00	3.25	3.50
RE	19.575	16.318	13.849
t	32.90	30.75	29.30
Z	0.181	0.218	0.258
pHS	4.330	4.430	4.524

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
11.694	9.766	8.486	7.568	6.655	5.826	5.540	5.004	4.571	4.246	4.095
28.21	27.43	23.30	23.07	22.87	22.73	26.65	26.59	26.56	22.95	22.94
0.307	0.370	0.431	0.485	0.554	0.636	0.669	0.744	0.817	0.891	0.925
4.627	4.747	4.855	4.948	5.067	5.214	5.278	5.433	5.618	5.878	6.056
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.978	3.900	3.817	3.793	3.777	3.766	3.813	3.808	3.803	3.797	3.804
22.93	22.92	33.63	33.62	33.61	33.60	22.89	22.90	22.91	22.93	22.98
0.953	0.972	0.987	0.992	0.996	0.997	0.998	0.999	0.999	1.000	1.000
6.269	6.501	6.833	7.071	7.316	7.564	7.738	7.987	8.236	8.486	8.740
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 12				
3.800	3.794	3.787	3.762	3.752	3.735					
23.06	23.21	23.49	31.60	33.11	36.50					
1.000	1.000	1.000	1.000	1.000	1.000					
8.991	9.243	9.496	9.832	10.096	10.375					

29 CAPROIC ACID (S) C6H1202

-1	30.2	4.857	116.16							

pHL	3.00	3.25	3.50
RE	13.156	10.992	9.364
t	26.15	24.73	23.76
Z	0.197	0.236	0.278
pHS	4.228	4.327	4.421

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.945	6.670	5.711	5.136	4.555	4.023	3.845	3.503	3.224	3.003	2.909
23.02	22.46	19.43	19.27	19.12	19.01	21.84	21.79	21.75	19.12	19.11
0.328	0.393	0.464	0.517	0.585	0.665	0.696	0.767	0.835	0.905	0.935
4.524	4.644	4.767	4.858	4.976	5.123	5.186	5.341	5.527	5.798	5.977
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.837	2.788	2.743	2.729	2.719	2.712	2.734	2.731	2.728	2.725	2.729
19.10	19.10	26.81	26.80	26.80	26.79	19.06	19.06	19.07	19.09	19.11
0.959	0.976	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.191	6.424	6.738	6.976	7.221	7.469	7.661	7.910	8.159	8.409	8.661
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.726	2.723	2.720	2.710	2.706	2.700					
19.15	19.23	19.36	24.89	25.49	26.69					
1.000	1.000	1.000	1.000	1.000	1.000					
8.912	9.162	9.414	9.721	9.977	10.239					

30 CAPRYLIC ACID C8H1602

-1	27.4	4.894	144.21							

pHL	3.00	3.25	3.50
RE	14.801	12.356	10.515
t	28.02	26.40	25.30
Z	0.193	0.232	0.273
pHS	4.255	4.355	4.449

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
8.909	7.469	6.428	5.767	5.103	4.497	4.293	3.902	3.586	3.340	3.232
24.46	23.83	20.50	20.32	20.16	20.03	23.17	23.11	23.08	20.17	20.16
0.323	0.388	0.455	0.509	0.578	0.658	0.690	0.762	0.831	0.902	0.933
4.552	4.672	4.790	4.883	5.001	5.148	5.211	5.367	5.553	5.820	6.000
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.149	3.093	3.039	3.022	3.011	3.003	3.031	3.028	3.024	3.020	3.025
20.15	20.15	28.69	28.68	28.67	28.67	20.11	20.12	20.12	20.14	20.17
0.958	0.975	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.213	6.446	6.766	7.004	7.250	7.498	7.684	7.932	8.182	8.431	8.684
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 7				
3.022	3.018	3.014	3.001	2.995	2.988					
20.22	20.31	20.48	26.68	27.47	29.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.935	9.186	9.438	9.753	10.011	10.276					

31 CARBONIC ACID H2CO3

-1	46.1	6.352	62.03				pHL	3.00	3.25	3.50
-2	71.8	10.329					RE	43.836	36.281	30.593
							t	19.64	19.01	18.56
							Z	0.038	0.045	0.054
							pHS	4.934	5.020	5.097

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
25.532	20.840	14.611	12.986	11.188	9.343	7.956	6.854	5.745	3.518	3.267
18.18	17.88	15.88	15.82	15.76	15.70	17.46	17.44	17.42	15.72	15.72
0.065	0.079	0.114	0.128	0.149	0.179	0.211	0.245	0.294	0.487	0.525
5.180	5.275	5.446	5.504	5.579	5.672	5.759	5.843	5.947	6.299	6.364

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.966	2.653	2.146	2.051	1.955	1.875	1.823	1.793	1.770	1.753	1.739
15.71	15.70	20.61	20.61	20.62	20.63	15.67	15.70	15.76	15.87	16.05
0.579	0.650	0.808	0.846	0.889	0.928	0.960	0.977	0.991	1.004	1.019
6.459	6.586	6.937	7.053	7.213	7.412	7.657	7.862	8.092	8.334	8.592

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 4
1.720	1.694	1.655	1.589	1.519	1.443	
16.37	16.90	17.75	22.86	24.69	26.87	
1.039	1.070	1.120	1.210	1.317	1.447	
8.839	9.088	9.338	9.625	9.861	10.097	

32 CHLORIC ACID (S) HClO3

-1	67.0	-2.700	84.46				pHL	3.00	3.25	3.50
							RE	1.186	1.186	1.186
							t	19.42	17.43	16.28
							Z	1.000	1.000	1.000
							pHS	3.052	3.293	3.534

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.186	1.185	1.186	1.186	1.186	1.186	1.186	1.186	1.186	1.187	1.186
15.63	15.25	14.06	13.85	13.73	13.66	14.92	14.88	14.86	13.70	13.69
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.778	4.026	4.027	4.272	4.521	4.770	4.775	5.024	5.274	5.520	5.770

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.186	1.186	1.186	1.186	1.185	1.185	1.186	1.186	1.186	1.186	1.186
13.69	13.69	17.05	17.05	17.05	17.05	13.67	13.67	13.67	13.68	13.68
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.020	6.270	6.530	6.780	7.030	7.280	7.520	7.770	8.020	8.270	8.520

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 4
1.186	1.186	1.186	1.186	1.185	1.185	
13.69	13.71	13.75	16.03	16.13	16.32	
1.000	1.000	1.000	1.000	1.000	1.000	
8.770	9.020	9.270	9.528	9.779	10.029	

33 2-CHLORO-3-OH-BUTYRIC ACID C4H7ClO3

-1	34.4	2.602	138.55				pHL	3.00	3.25	3.50
							RE	2.721	2.600	2.518
							t	27.09	24.49	22.81
							Z	0.866	0.907	0.938
							pHS	3.377	3.557	3.743

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.460	2.421	2.431	2.409	2.394	2.384	2.381	2.375	2.370	2.381	2.379
21.68	20.97	18.53	18.16	17.93	17.79	20.31	20.24	20.19	17.88	17.87
0.960	0.976	0.977	0.986	0.992	0.995	0.996	0.997	0.999	0.999	1.000
3.949	4.175	4.189	4.406	4.640	4.884	4.909	5.154	5.402	5.634	5.882

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.377	2.375	2.367	2.365	2.364	2.362	2.379	2.378	2.376	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.131	6.381	6.682	6.932	7.182	7.432	7.630	7.881	8.131	8.381	8.632

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.376	2.374	2.372	2.365	2.362	2.358	
17.89	17.95	18.06	22.80	23.24	24.08	
1.000	1.000	1.000	1.000	1.000	1.000	
8.883	9.133	9.385	9.682	9.936	10.195	

34 CHLOROACETIC ACID C2H3ClO2
-1 43.7 2.865 94.50

pHL	3.00	3.25	3.50
RE	2.356	2.189	2.073
t	22.92	21.04	19.81
Z	0.778	0.838	0.886
pHS	3.373	3.542	3.717

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.989	1.931	1.932	1.900	1.878	1.864	1.863	1.855	1.849	1.853	1.851
18.96	18.42	16.51	16.23	16.06	15.95	17.91	17.85	17.82	16.02	16.01
0.924	0.953	0.956	0.972	0.983	0.990	0.991	0.995	0.997	0.998	0.999
3.914	4.133	4.159	4.369	4.599	4.841	4.860	5.104	5.351	5.589	5.836

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.850	1.848	1.845	1.844	1.843	1.842	1.850	1.850	1.849	1.848	1.850
16.00	16.00	21.24	21.24	21.24	21.24	15.97	15.97	15.98	15.99	15.99
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.085	6.335	6.621	6.871	7.121	7.371	7.585	7.835	8.085	8.335	8.586

8.75	9.00	9.25	9.50	9.75	10.00
1.849	1.848	1.846	1.844	1.842	1.840
16.02	16.05	16.12	19.75	20.00	20.46
1.000	1.000	1.000	1.000	1.000	1.000
8.836	9.086	9.337	9.619	9.871	10.125

(Ref.) : 1

35 m-CHLOROBENZOIC ACID C7H5ClO2
-1 32.0 3.830 156.57

pHL	3.00	3.25	3.50
RE	5.244	4.571	4.066
t	26.31	24.55	23.34
Z	0.475	0.547	0.617
pHS	3.760	3.883	4.007

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.642	3.290	3.191	3.006	2.851	2.737	2.720	2.652	2.609	2.600	2.585
22.45	21.81	19.06	18.79	18.59	18.45	21.16	21.09	21.04	18.55	18.54
0.691	0.767	0.796	0.847	0.895	0.933	0.938	0.962	0.978	0.987	0.992
4.147	4.314	4.388	4.537	4.722	4.935	4.972	5.194	5.431	5.668	5.905

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.575	2.568	2.555	2.553	2.550	2.548	2.568	2.567	2.565	2.563	2.566
18.53	18.52	25.78	25.78	25.77	25.77	18.49	18.49	18.50	18.51	18.53
0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.149	6.397	6.704	6.953	7.202	7.452	7.646	7.896	8.146	8.396	8.648

8.75	9.00	9.25	9.50	9.75	10.00
2.564	2.562	2.559	2.551	2.547	2.542
18.57	18.64	18.76	23.92	24.44	25.46
1.000	1.000	1.000	1.000	1.000	1.000
8.898	9.149	9.401	9.704	9.959	10.219

(Ref.) : 2 , 1

36 o-CHLOROBENZOIC ACID C7H5ClO2
-1 33.8 2.943 156.57

pHL	3.00	3.25	3.50
RE	3.077	2.866	2.717
t	26.89	24.53	22.96
Z	0.777	0.836	0.883
pHS	3.452	3.615	3.785

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.606	2.528	2.534	2.491	2.461	2.441	2.437	2.426	2.418	2.428	2.425
21.88	21.17	18.67	18.32	18.09	17.95	20.52	20.44	20.39	18.04	18.03
0.922	0.951	0.954	0.971	0.982	0.990	0.990	0.994	0.997	0.998	0.999
3.977	4.193	4.217	4.423	4.650	4.890	4.917	5.160	5.407	5.639	5.886

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.422	2.419	2.411	2.409	2.408	2.406	2.424	2.422	2.421	2.419	2.422
18.02	18.02	24.87	24.87	24.86	24.86	17.98	17.98	17.99	18.00	18.02
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.135	6.384	6.688	6.937	7.187	7.437	7.634	7.884	8.134	8.384	8.636

8.75	9.00	9.25	9.50	9.75	10.00
2.420	2.418	2.416	2.409	2.406	2.402
18.05	18.11	18.22	23.07	23.52	24.40
1.000	1.000	1.000	1.000	1.000	1.000
8.886	9.137	9.388	9.687	9.942	10.200

(Ref.) : 2 , 1

37 p-CHLOROBENZOIC ACID C7H5ClO2
-1 33.4 3.977 156.57

pHL	3.00	3.25	3.50							
RE	5.625	4.857	4.280							
t	25.32	23.74	22.66							
Z	0.423	0.491	0.559							
pHS	3.815	3.934	4.050							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.791	3.375	3.223	3.011	2.824	2.682	2.659	2.574	2.517	2.498	2.478
21.84	21.26	18.60	18.37	18.18	18.06	20.64	20.57	20.53	18.15	18.14
0.633	0.713	0.752	0.807	0.862	0.909	0.916	0.947	0.968	0.982	0.989
4.183	4.340	4.426	4.563	4.736	4.940	4.980	5.194	5.426	5.667	5.899
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.466	2.457	2.445	2.442	2.439	2.437	2.455	2.453	2.452	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.994	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.142	6.389	6.693	6.941	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

38 2-CHLOROBUTYRIC ACID C4H7ClO2
-1 34.4 2.839 122.55

pHL	3.00	3.25	3.50							
RE	2.916	2.738	2.613							
t	26.74	24.33	22.75							
Z	0.806	0.860	0.902							
pHS	3.423	3.592	3.767							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.522	2.459	2.467	2.431	2.407	2.392	2.388	2.379	2.373	2.382	2.380
21.66	20.96	18.52	18.16	17.93	17.79	20.31	20.24	20.19	17.88	17.87
0.936	0.960	0.962	0.976	0.986	0.992	0.992	0.996	0.998	0.999	0.999
3.964	4.183	4.205	4.414	4.644	4.886	4.912	5.155	5.403	5.635	5.882
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.377	2.375	2.367	2.365	2.364	2.362	2.379	2.378	2.376	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.131	6.381	6.682	6.932	7.182	7.432	7.631	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

39 3-CHLOROBUTYRIC ACID C4H7ClO2
-1 34.4 4.056 122.55

pHL	3.00	3.25	3.50							
RE	5.824	5.006	4.391							
t	24.70	23.23	22.22							
Z	0.395	0.461	0.527							
pHS	3.846	3.961	4.075							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.867	3.418	3.230	3.005	2.802	2.643	2.617	2.521	2.456	2.430	2.408
21.45	20.89	18.30	18.09	17.92	17.79	20.30	20.23	20.19	17.88	17.87
0.601	0.682	0.727	0.783	0.842	0.894	0.902	0.937	0.962	0.978	0.987
4.203	4.355	4.447	4.579	4.745	4.943	4.984	5.193	5.422	5.667	5.895
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.394	2.384	2.371	2.368	2.365	2.363	2.380	2.378	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.137	6.383	6.686	6.934	7.182	7.432	7.631	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

40 2-CHLOROCROTONIC ACID C4H5ClO2

-1 35.4 3.155 120.54

pHL	3.00	3.25	3.50
RE	3.225	2.947	2.746
t	25.70	23.63	22.24
Z	0.704	0.773	0.831
pHS	3.499	3.652	3.811

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.592	2.479	2.476	2.414	2.369	2.340	2.336	2.319	2.308	2.315	2.311
21.27	20.61	18.21	17.89	17.68	17.55	19.99	19.92	19.88	17.63	17.62
0.882	0.923	0.929	0.953	0.971	0.983	0.984	0.991	0.995	0.997	0.998
3.991	4.197	4.232	4.427	4.648	4.885	4.911	5.152	5.398	5.631	5.877
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.308	2.305	2.297	2.296	2.294	2.293	2.308	2.307	2.306	2.304	2.307
17.61	17.61	24.14	24.14	24.13	24.13	17.57	17.58	17.58	17.59	17.61
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.126	6.375	6.675	6.925	7.174	7.424	7.625	7.875	8.125	8.375	8.626
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.305	2.304	2.301	2.296	2.293	2.289					
17.64	17.70	17.79	22.39	22.80	23.57					
1.000	1.000	1.000	1.000	1.000	1.000					
8.877	9.127	9.379	9.674	9.928	10.186					

41 3-CHLOROCROTONIC ACID C4H5ClO2

-1 35.4 3.848 120.54

pHL	3.00	3.25	3.50
RE	4.865	4.227	3.750
t	24.52	22.98	21.93
Z	0.461	0.532	0.602
pHS	3.753	3.875	3.997

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.348	3.013	2.905	2.732	2.585	2.475	2.459	2.394	2.352	2.340	2.326
21.14	20.57	18.08	17.85	17.67	17.55	19.98	19.92	19.87	17.63	17.62
0.676	0.754	0.787	0.838	0.887	0.928	0.933	0.958	0.975	0.986	0.992
4.135	4.300	4.380	4.525	4.707	4.917	4.953	5.173	5.408	5.649	5.884
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.316	2.310	2.300	2.297	2.295	2.293	2.309	2.307	2.306	2.304	2.307
17.61	17.61	24.14	24.14	24.13	24.13	17.57	17.58	17.58	17.59	17.61
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.129	6.376	6.677	6.925	7.175	7.424	7.625	7.875	8.125	8.375	8.626
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.305	2.304	2.301	2.296	2.293	2.289					
17.64	17.70	17.79	22.39	22.80	23.57					
1.000	1.000	1.000	1.000	1.000	1.000					
8.877	9.127	9.379	9.674	9.928	10.186					

42 CHLORODIBROMOACETIC ACID C2HBr2ClO2

-1 36.5 1.000 252.29

pHL	3.00	3.25	3.50
RE	2.235	2.231	2.228
t	26.84	23.91	22.11
Z	0.995	0.997	0.998
pHS	3.264	3.474	3.686

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.226	2.225	2.234	2.233	2.232	2.230	2.228	2.227	2.225	2.235	2.234
20.97	20.28	18.02	17.64	17.42	17.29	19.66	19.59	19.55	17.37	17.36
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.911	4.148	4.152	4.382	4.623	4.869	4.892	5.139	5.388	5.620	5.869
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.233	2.231	2.224	2.224	2.222	2.221	2.235	2.234	2.233	2.231	2.234
17.35	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.119	6.368	6.666	6.916	7.166	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

43 CHLORODIFLUOROACETIC ACID C2HClF2O2

-1 38.6 1.000 130.48

pHL	3.00	3.25	3.50
RE	2.109	2.105	2.102
t	25.94	23.13	21.40
Z	0.995	0.997	0.998
pHS	3.244	3.456	3.671

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.100	2.099	2.107	2.106	2.105	2.103	2.102	2.100	2.099	2.107	2.106
20.32	19.67	17.53	17.18	16.97	16.85	19.08	19.01	18.97	16.92	16.91
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.897	4.135	4.139	4.370	4.611	4.858	4.879	5.127	5.376	5.609	5.858
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.105	2.104	2.098	2.098	2.097	2.095	2.107	2.107	2.106	2.104	2.106
16.91	16.90	22.87	22.86	22.86	22.86	16.87	16.87	16.88	16.89	16.90
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.108	6.358	6.652	6.902	7.152	7.401	7.608	7.858	8.108	8.358	8.609
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12				
2.105	2.104	2.102	2.098	2.095	2.093					
16.93	16.97	17.06	21.22	21.56	22.18					
1.000	1.000	1.000	1.000	1.000	1.000					
8.859	9.110	9.361	9.650	9.903	10.159					

44 2-CHLOROISOCROTONIC ACID C4H5ClO2

-1 35.4 2.810 120.54

pHL	3.00	3.25	3.50
RE	2.812	2.643	2.526
t	26.28	23.92	22.36
Z	0.811	0.865	0.906
pHS	3.409	3.580	3.757

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.441	2.382	2.390	2.357	2.334	2.320	2.317	2.308	2.302	2.311	2.309
21.30	20.62	18.25	17.90	17.68	17.55	19.99	19.92	19.88	17.63	17.62
0.938	0.962	0.964	0.977	0.987	0.992	0.993	0.996	0.998	0.999	0.999
3.955	4.175	4.196	4.407	4.638	4.879	4.904	5.149	5.396	5.629	5.876
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.307	2.304	2.297	2.296	2.294	2.292	2.308	2.307	2.306	2.304	2.307
17.61	17.61	24.14	24.14	24.13	24.13	17.57	17.58	17.58	17.59	17.61
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.125	6.375	6.675	6.924	7.174	7.424	7.625	7.875	8.125	8.375	8.626
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.305	2.304	2.301	2.296	2.293	2.289					
17.64	17.70	17.79	22.39	22.80	23.57					
1.000	1.000	1.000	1.000	1.000	1.000					
8.877	9.127	9.379	9.674	9.928	10.186					

45 m-CHLOROPHENOL C6H5ClO

-1 33.4 9.023 128.56

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	□□□□□□
t	23.86	22.87	22.17
Z	0.002	0.002	0.003
pHS	6.286	6.373	6.451

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	61.200	55.694
21.62	21.18	18.44	18.35	18.27	18.20	20.61	20.58	20.56	18.30	18.30
0.003	0.004	0.006	0.007	0.008	0.010	0.012	0.014	0.017	0.037	0.041
6.534	6.626	6.786	6.843	6.914	7.001	7.089	7.164	7.255	7.602	7.644
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
48.789	41.096	18.793	17.288	15.352	13.145	7.802	7.185	6.417	5.579	4.249
18.29	18.29	24.92	24.93	24.94	24.95	18.27	18.27	18.28	18.29	18.33
0.047	0.056	0.123	0.134	0.151	0.176	0.302	0.328	0.369	0.425	0.564
7.704	7.782	8.155	8.197	8.257	8.337	8.637	8.689	8.765	8.866	9.106
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
3.850	3.456	3.119	2.800	2.659	2.562					
18.37	18.43	18.54	23.51	23.98	24.91					
0.625	0.698	0.776	0.866	0.912	0.947					
9.213	9.354	9.527	9.798	10.005	10.237					

46 o-CHLOROPHENOL C6H5Cl0
-1 33.4 8.477 128.56

pHL	3.00	3.25	3.50							
RE										
t	23.80	22.80	22.10							
Z	0.003	0.004	0.005							
pHS	6.013	6.099	6.177							
	3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
								88.132	71.708	33.661	30.647
	21.54	21.11	18.37	18.28	18.20	18.13	20.53	20.51	20.48	18.22	18.22
	0.006	0.008	0.011	0.012	0.015	0.018	0.022	0.026	0.032	0.068	0.075
	6.260	6.353	6.513	6.569	6.641	6.729	6.816	6.892	6.984	7.330	7.374
	6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
	26.879	22.697	11.020	10.152	9.048	7.807	5.171	4.789	4.330	3.852	3.255
	18.21	18.21	24.87	24.88	24.89	24.90	18.17	18.17	18.17	18.18	18.20
	0.085	0.101	0.211	0.230	0.258	0.300	0.461	0.499	0.553	0.624	0.744
	7.435	7.516	7.887	7.933	7.999	8.088	8.382	8.447	8.540	8.666	8.907
	8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
	3.026	2.826	2.678	2.559	2.506	2.471					
	18.23	18.29	18.40	23.33	23.80	24.70					
	0.803	0.861	0.910	0.951	0.971	0.983					
	9.051	9.232	9.443	9.729	9.964	10.214					

47 p-CHLOROPHENOL C6H5Cl0
-1 33.4 9.378 128.60

pHL	3.00	3.25	3.50							
RE										
t	23.98	23.00	22.31							
Z	0.001	0.001	0.002							
pHS	6.465	6.552	6.630							
	3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
										90.705	82.548
	21.76	21.32	18.56	18.48	18.40	18.33	20.74	20.72	20.70	18.43	18.43
	0.002	0.003	0.004	0.004	0.005	0.006	0.008	0.009	0.011	0.025	0.028
	6.712	6.805	6.965	7.022	7.093	7.179	7.267	7.342	7.432	7.781	7.822
	6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
	72.299	60.855	27.121	24.943	22.127	18.897	10.628	9.768	8.685	7.481	5.343
	18.43	18.42	25.07	25.07	25.08	25.10	18.42	18.43	18.44	18.45	18.52
	0.031	0.037	0.085	0.092	0.104	0.122	0.220	0.240	0.270	0.315	0.445
	7.881	7.959	8.332	8.372	8.430	8.507	8.809	8.857	8.925	9.017	9.256
	8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
	4.788	4.211	3.687	3.120	2.884	2.705					
	18.56	18.63	18.75	23.80	24.30	25.26					
	0.498	0.569	0.652	0.773	0.838	0.894					
	9.347	9.468	9.618	9.878	10.059	10.271					

48 p-CHLOROPHENYLACETIC ACID C8H7Cl02
-1 34.5 4.190 170.60

pHL	3.00	3.25	3.50							
RE	6.462	5.519	4.810							
t	24.48	23.08	22.12							
Z	0.354	0.416	0.478							
pHS	3.905	4.017	4.125							
	3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
	4.202	3.673	3.414	3.155	2.914	2.718	2.682	2.562	2.479	2.439	2.411
	21.38	20.84	18.24	18.05	17.89	17.77	20.26	20.20	20.16	17.86	17.84
	0.550	0.631	0.684	0.742	0.805	0.865	0.876	0.919	0.950	0.971	0.982
	4.247	4.392	4.493	4.615	4.771	4.960	5.005	5.205	5.429	5.677	5.900
	6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
	2.392	2.380	2.366	2.362	2.359	2.356	2.372	2.371	2.370	2.367	2.370
	17.84	17.83	24.54	24.54	24.53	24.53	17.80	17.80	17.81	17.82	17.83
	0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
	6.138	6.384	6.687	6.933	7.182	7.431	7.630	7.880	8.130	8.380	8.632
	8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2				
	2.369	2.367	2.364	2.358	2.355	2.351					
	17.87	17.93	18.03	22.76	23.20	24.02					
	1.000	1.000	1.000	1.000	1.000	1.000					
	8.882	9.133	9.384	9.681	9.936	10.194					

49 2-CHLOROPROPIONIC ACID C3H5ClO2

-1	36.9	2.796	108.52				pHL	3.00	3.25	3.50
							RE	2.692	2.530	2.418
							t	25.60	23.32	21.82
							Z	0.812	0.865	0.906
							pHS	3.396	3.567	3.746
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.337	2.281	2.287	2.256	2.234	2.221	2.218	2.210	2.204	2.212	2.210
20.80	20.15	17.88	17.54	17.33	17.20	19.54	19.47	19.43	17.28	17.27
0.939	0.962	0.964	0.978	0.987	0.992	0.993	0.996	0.998	0.999	0.999
3.945	4.165	4.186	4.398	4.629	4.871	4.895	5.139	5.387	5.620	5.868
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.208	2.206	2.200	2.199	2.197	2.195	2.210	2.209	2.208	2.206	2.208
17.26	17.26	23.52	23.51	23.51	23.50	17.23	17.23	17.24	17.25	17.26
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.117	6.366	6.664	6.913	7.163	7.413	7.616	7.866	8.116	8.366	8.618
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.207	2.205	2.203	2.198	2.196	2.193					
17.29	17.34	17.43	21.82	22.18	22.88					
1.000	1.000	1.000	1.000	1.000	1.000					
8.868	9.119	9.370	9.662	9.916	10.173					

50 3-CHLOROPROPIONIC ACID C3H5ClO2

-1	36.9	3.867	108.52				pHL	3.00	3.25	3.50
							RE	4.756	4.125	3.653
							t	23.82	22.38	21.39
							Z	0.452	0.522	0.592
							pHS	3.756	3.877	3.997
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.255	2.922	2.806	2.636	2.489	2.379	2.364	2.299	2.256	2.242	2.227
20.64	20.10	17.71	17.49	17.32	17.20	19.53	19.47	19.43	17.28	17.27
0.666	0.744	0.780	0.831	0.882	0.924	0.929	0.956	0.974	0.985	0.991
4.134	4.297	4.380	4.524	4.703	4.911	4.947	5.165	5.400	5.643	5.877
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.218	2.212	2.202	2.200	2.198	2.196	2.210	2.209	2.208	2.206	2.208
17.27	17.26	23.51	23.51	23.51	23.50	17.23	17.23	17.24	17.25	17.26
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.121	6.368	6.666	6.914	7.164	7.413	7.617	7.866	8.116	8.367	8.618
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.207	2.205	2.203	2.198	2.196	2.193					
17.29	17.34	17.43	21.82	22.18	22.88					
1.000	1.000	1.000	1.000	1.000	1.000					
8.868	9.119	9.370	9.662	9.916	10.173					

51 CHLOROUS ACID HClO2

-1	53.9	1.960	68.46				pHL	3.00	3.25	3.50
							RE	1.566	1.534	1.514
							t	21.27	19.19	17.93
							Z	0.946	0.967	0.980
							pHS	3.166	3.380	3.598
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.501	1.493	1.496	1.492	1.489	1.487	1.487	1.485	1.484	1.487	1.487
17.15	16.69	15.18	14.93	14.78	14.69	16.27	16.22	16.20	14.74	14.74
0.988	0.993	0.993	0.996	0.998	0.999	0.999	0.999	1.000	1.000	1.000
3.828	4.068	4.075	4.310	4.554	4.801	4.812	5.061	5.310	5.552	5.801
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.486	1.485	1.484	1.484	1.483	1.483	1.487	1.486	1.486	1.486	1.486
14.73	14.73	18.94	18.94	18.94	18.94	14.71	14.71	14.71	14.72	14.72
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.051	6.300	6.573	6.823	7.073	7.323	7.550	7.800	8.050	8.300	8.551
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 4				
1.486	1.485	1.485	1.484	1.483	1.482					
14.74	14.77	14.81	17.70	17.86	18.15					
1.000	1.000	1.000	1.000	1.000	1.000					
8.801	9.051	9.302	9.571	9.822	10.074					

52 5-CHLOROVALERIC ACID C5H9ClO2

-1	32.3	4.697	136.58

pHL	3.00	3.25	3.50
RE	10.670	8.952	7.661
t	25.08	23.75	22.84
Z	0.227	0.271	0.318
pHS	4.145	4.247	4.343

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.536	5.529	4.812	4.354	3.894	3.481	3.359	3.095	2.887	2.736	2.666
22.13	21.60	18.78	18.62	18.47	18.36	21.01	20.95	20.92	18.46	18.45
0.374	0.444	0.515	0.571	0.640	0.718	0.745	0.811	0.871	0.926	0.951
4.449	4.573	4.694	4.791	4.915	5.071	5.130	5.294	5.490	5.756	5.947
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.615	2.581	2.549	2.539	2.532	2.526	2.545	2.543	2.540	2.538	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.970	0.982	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.168	6.405	6.715	6.955	7.202	7.450	7.646	7.895	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

53 CHROMIC ACID H2CrO4

-1	59.3	0.745	118.01
-2	81.1	6.490	

pHL	3.00	3.25	3.50
RE	1.350	1.347	1.346
t	20.55	18.43	17.20
Z	0.997	0.999	1.000
pHS	3.095	3.328	3.562

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.344	1.343	1.345	1.343	1.340	1.336	1.335	1.327	1.315	1.294	1.266
16.49	16.10	14.74	14.55	14.52	14.62	16.08	16.36	16.88	16.45	17.62
1.002	1.004	1.004	1.008	1.015	1.026	1.027	1.047	1.080	1.146	1.230
3.802	4.047	4.050	4.293	4.540	4.789	4.800	5.049	5.299	5.587	5.825
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.230	1.190	1.140	1.114	1.092	1.076	1.074	1.068	1.065	1.062	1.062
19.10	20.75	28.02	29.31	30.35	31.08	25.71	25.95	26.10	26.19	26.24
1.342	1.475	1.647	1.748	1.835	1.898	1.940	1.965	1.980	1.988	1.993
6.062	6.299	6.601	6.809	7.037	7.275	7.527	7.768	8.015	8.263	8.513
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 2				
1.061	1.060	1.060	1.055	1.055	1.054					
26.29	26.33	26.40	30.41	30.58	30.88					
1.996	1.998	1.999	1.999	2.000	2.000					
8.763	9.013	9.262	9.515	9.765	10.015					

54 CINNAMIC ACID C9H8O2

-1	28.3	4.438	148.16

pHL	3.00	3.25	3.50
RE	9.443	7.998	6.906
t	27.82	26.11	24.95
Z	0.296	0.350	0.407
pHS	4.040	4.147	4.250

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.962	5.130	4.685	4.278	3.890	3.562	3.484	3.279	3.131	3.052	3.001
24.07	23.43	20.23	20.01	19.83	19.69	22.75	22.68	22.64	19.82	19.80
0.473	0.552	0.611	0.671	0.740	0.811	0.828	0.882	0.924	0.956	0.973
4.366	4.501	4.604	4.716	4.860	5.036	5.088	5.276	5.491	5.739	5.952
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.966	2.943	2.916	2.909	2.903	2.899	2.926	2.924	2.921	2.918	2.923
19.79	19.79	28.04	28.04	28.03	28.02	19.75	19.75	19.76	19.78	19.80
0.984	0.991	0.995	0.997	0.999	0.999	0.999	1.000	1.000	1.000	1.000
6.186	6.429	6.745	6.990	7.238	7.487	7.674	7.924	8.174	8.424	8.676
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.920	2.917	2.913	2.901	2.896	2.889					
19.85	19.94	20.09	26.06	26.78	28.24					
1.000	1.000	1.000	1.000	1.000	1.000					
8.927	9.178	9.430	9.742	10.000	10.263					

55 cis-CINNAMIC ACID C9H802

-1	28.3	3.879	148.16				pHL	3.00	3.25	3.50
							RE	6.035	5.258	4.673
							t	28.66	26.63	25.26
							Z	0.469	0.540	0.609
							pHS	3.799	3.921	4.043

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.181	3.771	3.662	3.444	3.261	3.125	3.103	3.023	2.972	2.963	2.945
24.23	23.51	20.38	20.08	19.85	19.70	22.78	22.70	22.65	19.82	19.80
0.683	0.760	0.789	0.841	0.890	0.930	0.935	0.960	0.977	0.986	0.992
4.183	4.349	4.419	4.568	4.751	4.963	5.004	5.226	5.462	5.696	5.932
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.933	2.925	2.907	2.904	2.900	2.897	2.925	2.923	2.921	2.918	2.923
19.79	19.79	28.05	28.04	28.03	28.02	19.75	19.75	19.76	19.78	19.80
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.177	6.425	6.739	6.988	7.237	7.487	7.674	7.924	8.174	8.424	8.676
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.920	2.917	2.913	2.901	2.896	2.889					
19.85	19.94	20.09	26.06	26.78	28.24					
1.000	1.000	1.000	1.000	1.000	1.000					
8.927	9.178	9.430	9.742	10.000	10.263					

56 CITRACONIC ACID C5H604

-1	28.0	2.458	130.10				pHL	3.00	3.25	3.50
-2	56.0	6.146					RE	3.215	3.113	3.041
							t	31.42	28.21	26.16
							Z	0.910	0.941	0.964
							pHS	3.419	3.602	3.790

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.985	2.938	2.954	2.910	2.852	2.770	2.750	2.631	2.474	2.234	2.087
24.82	24.05	21.03	20.76	20.80	21.16	24.40	25.14	26.20	25.14	26.17
0.983	1.000	1.001	1.017	1.038	1.071	1.077	1.130	1.208	1.362	1.467
3.997	4.224	4.240	4.458	4.692	4.934	4.974	5.212	5.447	5.772	5.956
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.946	1.825	1.700	1.651	1.615	1.591	1.599	1.591	1.585	1.581	1.582
27.17	28.03	37.63	37.99	38.24	38.39	29.67	29.73	29.77	29.80	29.83
1.584	1.699	1.826	1.884	1.928	1.957	1.975	1.985	1.992	1.995	1.997
6.156	6.370	6.680	6.883	7.110	7.349	7.577	7.819	8.066	8.315	8.566
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 2				
1.580	1.577	1.575	1.566	1.563	1.560					
29.86	29.92	30.01	36.07	36.40	37.03					
1.998	1.999	2.000	2.000	2.000	2.000					
8.815	9.065	9.315	9.587	9.838	10.091					

57 CITRIC ACID (S) C6H807

-1	28.7	3.128	192.13				pHL	3.00	3.25	3.50
-2	54.7	4.761					RE	3.601	3.244	2.958
-3	74.4	6.396					t	31.06	28.91	27.81
							Z	0.796	0.889	0.984
							pHS	3.529	3.683	3.842

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.698	2.454	2.396	2.212	2.037	1.883	1.859	1.744	1.649	1.573	1.511
27.49	27.90	25.15	26.00	27.08	28.28	31.80	33.01	34.33	32.98	34.50
1.090	1.215	1.260	1.384	1.527	1.679	1.701	1.843	1.984	2.156	2.296
4.021	4.220	4.286	4.465	4.664	4.878	4.912	5.126	5.354	5.632	5.849
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.452	1.400	1.341	1.314	1.294	1.281	1.302	1.297	1.293	1.290	1.293
36.15	37.73	49.56	50.49	51.13	51.52	41.22	41.35	41.43	41.48	41.53
2.450	2.601	2.749	2.837	2.900	2.941	2.965	2.980	2.989	2.994	2.996
6.078	6.314	6.599	6.825	7.063	7.307	7.546	7.793	8.041	8.291	8.541
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.291	1.289	1.286	1.273	1.270	1.266					
41.57	41.63	41.73	48.97	49.29	49.89					
2.998	2.999	2.999	3.000	3.000	3.000					
8.791	9.041	9.291	9.552	9.802	10.052					

58 CRESOL -1 33.4 7.377 C7H80 108.14

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	□□□□□□
t	23.80	22.79	22.08
Z	0.012	0.015	0.018
pHS	5.463	5.550	5.629

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	85.181	60.064	52.789	44.885	36.899	30.724	25.974	21.256	10.974	10.027
21.52	21.08	18.34	18.25	18.17	18.09	20.52	20.49	20.47	18.18	18.17
0.021	0.027	0.038	0.043	0.051	0.062	0.075	0.088	0.108	0.213	0.233
5.712	5.806	5.964	6.022	6.096	6.186	6.272	6.351	6.447	6.790	6.841

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
8.860	7.590	4.643	4.319	3.931	3.533	3.047	2.897	2.752	2.637	2.558
18.17	18.16	24.94	24.95	24.96	24.98	18.10	18.11	18.11	18.12	18.14
0.265	0.310	0.513	0.553	0.609	0.679	0.798	0.841	0.886	0.926	0.957
6.912	7.007	7.372	7.441	7.540	7.672	7.938	8.063	8.232	8.436	8.685

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.514	2.485	2.467	2.450	2.442	2.435	
18.17	18.23	18.34	23.25	23.72	24.63	
0.974	0.985	0.991	0.996	0.998	0.999	
8.910	9.149	9.396	9.694	9.947	10.205	

59 m-CRESOL -1 33.4 7.770 C7H80 108.14

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	□□□□□□
t	23.79	22.78	22.08
Z	0.008	0.009	0.011
pHS	5.659	5.746	5.824

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	93.326	81.981	69.643	57.161	47.317	39.934	32.584	16.066	14.652
21.52	21.09	18.34	18.26	18.17	18.10	20.52	20.49	20.47	18.19	18.18
0.014	0.017	0.024	0.028	0.033	0.040	0.048	0.057	0.070	0.144	0.158
5.908	6.001	6.160	6.217	6.290	6.378	6.465	6.543	6.637	6.981	7.028

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
12.898	10.969	6.067	5.616	5.058	4.457	3.512	3.298	3.068	2.861	2.686
18.18	18.18	24.90	24.91	24.93	24.94	18.12	18.12	18.12	18.13	18.15
0.180	0.213	0.389	0.421	0.469	0.534	0.688	0.734	0.791	0.850	0.910
7.095	7.182	7.551	7.608	7.690	7.802	8.081	8.178	8.314	8.488	8.735

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.597	2.535	2.496	2.464	2.450	2.439	
18.18	18.24	18.35	23.26	23.73	24.64	
0.941	0.964	0.979	0.989	0.994	0.997	
8.936	9.163	9.403	9.699	9.949	10.206	

60 p-CRESOL -1 33.4 7.959 C7H80 108.14

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	□□□□□□
t	23.79	22.78	22.08
Z	0.006	0.008	0.009
pHS	5.753	5.840	5.919

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	□□□□□□	□□□□□□	86.177	70.693	58.401	49.261	40.153	19.470	17.746
21.52	21.09	18.34	18.26	18.18	18.10	20.52	20.49	20.47	18.19	18.19
0.011	0.014	0.020	0.022	0.026	0.032	0.039	0.046	0.057	0.119	0.130
6.002	6.095	6.254	6.311	6.384	6.472	6.559	6.636	6.729	7.074	7.120

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
15.601	13.234	7.023	6.490	5.824	5.095	3.830	3.580	3.299	3.034	2.785
18.19	18.18	24.89	24.90	24.91	24.93	18.13	18.13	18.13	18.14	18.16
0.149	0.175	0.335	0.363	0.406	0.465	0.629	0.675	0.734	0.800	0.876
7.185	7.270	7.639	7.692	7.769	7.873	8.157	8.243	8.365	8.525	8.770

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.667	2.579	2.522	2.478	2.458	2.444	
18.19	18.25	18.35	23.27	23.74	24.65	
0.916	0.947	0.969	0.984	0.991	0.995	
8.957	9.174	9.409	9.703	9.951	10.207	

61 CROTONIC ACID C4H6O2
-1 33.5 4.705 86.09

	3.00	3.25	3.50
pHL	3.00	3.25	3.50
RE	10.417	8.738	7.476
t	24.46	23.20	22.33
Z	0.224	0.268	0.314
pHS	4.146	4.247	4.343

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.377	5.392	4.671	4.226	3.779	3.374	3.254	2.995	2.790	2.638	2.569
21.66	21.15	18.43	18.27	18.14	18.03	20.58	20.52	20.49	18.12	18.11
0.369	0.438	0.511	0.566	0.635	0.713	0.740	0.806	0.867	0.924	0.949
4.448	4.571	4.695	4.790	4.913	5.067	5.127	5.289	5.484	5.753	5.941

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.518	2.485	2.454	2.444	2.437	2.432	2.449	2.447	2.445	2.442	2.445
18.10	18.10	25.01	25.01	25.00	25.00	18.06	18.06	18.07	18.08	18.10
0.969	0.982	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.161	6.398	6.705	6.946	7.192	7.440	7.638	7.887	8.136	8.386	8.638

8.75	9.00	9.25	9.50	9.75	10.00
2.443	2.441	2.438	2.432	2.428	2.424
18.13	18.20	18.30	23.20	23.67	24.56
1.000	1.000	1.000	1.000	1.000	1.000
8.888	9.139	9.390	9.690	9.944	10.203

(Ref.) : 11 , 7

62 CYANIC ACID HCNO
-1 67.0 3.470 43.03

	3.00	3.25	3.50
pHL	3.00	3.25	3.50
RE	2.136	1.878	1.690
t	17.37	16.54	15.98
Z	0.548	0.625	0.695
pHS	3.519	3.655	3.791

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.538	1.416	1.379	1.318	1.269	1.235	1.233	1.214	1.202	1.195	1.192
15.55	15.24	13.96	13.83	13.73	13.67	14.92	14.88	14.86	13.70	13.69
0.766	0.833	0.857	0.898	0.933	0.959	0.960	0.976	0.986	0.992	0.996
3.946	4.127	4.207	4.372	4.571	4.795	4.812	5.041	5.282	5.536	5.776

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.189	1.188	1.187	1.186	1.186	1.185	1.187	1.186	1.186	1.186	1.186
13.69	13.69	17.05	17.05	17.05	17.05	13.67	13.67	13.67	13.68	13.68
0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.022	6.271	6.532	6.780	7.030	7.280	7.520	7.770	8.020	8.270	8.520

8.75	9.00	9.25	9.50	9.75	10.00
1.186	1.186	1.186	1.186	1.185	1.185
13.69	13.71	13.75	16.03	16.13	16.32
1.000	1.000	1.000	1.000	1.000	1.000
8.770	9.020	9.270	9.528	9.779	10.029

(Ref.) : 2 , 4

63 CYANOACETIC ACID C3H3NO2
-1 45.0 2.469 85.06

	3.00	3.25	3.50
pHL	3.00	3.25	3.50
RE	2.035	1.947	1.889
t	23.06	20.93	19.58
Z	0.876	0.916	0.945
pHS	3.281	3.470	3.667

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.850	1.824	1.828	1.814	1.804	1.798	1.797	1.794	1.791	1.796	1.794
18.70	18.16	16.33	16.04	15.86	15.76	17.66	17.60	17.57	15.82	15.81
0.966	0.980	0.980	0.988	0.993	0.996	0.996	0.998	0.999	0.999	1.000
3.881	4.112	4.126	4.349	4.587	4.832	4.849	5.096	5.344	5.582	5.830

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.794	1.792	1.789	1.789	1.788	1.787	1.794	1.794	1.793	1.792	1.794
15.81	15.81	20.89	20.89	20.88	20.88	15.78	15.78	15.78	15.79	15.80
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.080	6.330	6.614	6.864	7.114	7.364	7.580	7.830	8.080	8.330	8.580

8.75	9.00	9.25	9.50	9.75	10.00
1.793	1.792	1.791	1.788	1.787	1.785
15.82	15.86	15.92	19.43	19.67	20.10
1.000	1.000	1.000	1.000	1.000	1.000
8.831	9.081	9.332	9.611	9.864	10.117

(Ref.) : 1

64 m-CYANOBENZOIC ACID C8H5NO2

-1	31.3	3.598	147.13				pHL	3.00	3.25	3.50
							RE	4.581	4.058	3.668
							t	27.13	25.14	23.80
							Z	0.559	0.633	0.703
							pHS	3.673	3.805	3.940

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.349	3.094	3.051	2.913	2.805	2.729	2.718	2.674	2.647	2.648	2.638
22.81	22.12	19.34	19.03	18.81	18.67	21.44	21.36	21.31	18.77	18.75
0.772	0.838	0.855	0.897	0.932	0.959	0.961	0.977	0.987	0.992	0.996
4.094	4.276	4.333	4.500	4.700	4.924	4.959	5.190	5.431	5.665	5.906
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.631	2.626	2.614	2.612	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.153	6.401	6.709	6.959	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 7				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

65 CYCLOBUTANE-1,1-DICARBOXYLIC ACID C6H8O4

-1	25.5	3.127	144.13				pHL	3.00	3.25	3.50
-2	51.1	5.879					RE	4.258	3.935	3.696
							t	32.64	29.71	27.80
							Z	0.753	0.817	0.872
							pHS	3.567	3.721	3.881

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.502	3.343	3.343	3.223	3.090	2.932	2.894	2.708	2.503	2.253	2.119
26.52	25.81	22.46	22.34	22.59	23.23	26.90	27.93	29.16	27.68	28.54
0.922	0.968	0.976	1.015	1.061	1.122	1.136	1.220	1.329	1.506	1.611
4.064	4.272	4.308	4.505	4.726	4.959	5.005	5.230	5.454	5.760	5.941
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.999	1.905	1.815	1.780	1.756	1.739	1.758	1.753	1.748	1.745	1.747
29.30	29.90	40.12	40.34	40.48	40.54	30.88	30.91	30.93	30.95	30.98
1.717	1.810	1.895	1.934	1.961	1.977	1.986	1.992	1.996	1.998	1.999
6.145	6.366	6.667	6.886	7.122	7.366	7.587	7.832	8.081	8.330	8.581
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
1.745	1.742	1.740	1.728	1.724	1.720					
31.01	31.08	31.19	37.90	38.31	39.08					
1.999	2.000	2.000	2.000	2.000	2.000					
8.831	9.081	9.331	9.609	9.860	10.113					

66 CYCLOHEXANE-1,1-DICARBOXYLIC ACID C8H12O4

-1	24.0	3.451	172.18				pHL	3.00	3.25	3.50
-2	48.0	4.110					RE	3.966	3.398	2.971
							t	37.68	35.67	34.61
							Z	0.877	1.032	1.191
							pHS	3.607	3.737	3.871

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.623	2.348	2.309	2.160	2.046	1.970	1.958	1.914	1.886	1.891	1.881
34.13	34.08	30.53	30.70	30.91	31.10	35.02	35.14	35.22	31.78	31.80
1.362	1.535	1.581	1.701	1.804	1.880	1.886	1.932	1.961	1.977	1.987
4.025	4.206	4.260	4.432	4.636	4.863	4.887	5.120	5.362	5.603	5.846
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.874	1.869	1.852	1.849	1.846	1.842	1.873	1.871	1.869	1.866	1.871
31.81	31.82	42.27	42.26	42.23	42.20	31.80	31.80	31.81	31.81	31.84
1.993	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000	2.000
6.093	6.342	6.628	6.877	7.127	7.376	7.591	7.841	8.091	8.341	8.592
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
1.868	1.866	1.863	1.849	1.845	1.840					
31.88	31.95	32.07	39.28	39.75	40.64					
2.000	2.000	2.000	2.000	2.000	2.000					
8.842	9.092	9.343	9.624	9.876	10.130					

67 CYCLOPENTANE-1,1-DICARBOXYLIC ACID C7H1004 158.15

-1	25.0	3.230					pHL	3.00	3.25	3.50
-2	50.0	4.080					RE	3.506	3.052	2.706
							t	36.94	34.89	33.84
							Z	0.953	1.104	1.256
							pHS	3.540	3.682	3.828

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.421	2.196	2.170	2.041	1.943	1.877	1.867	1.827	1.802	1.807	1.798
33.40	33.40	30.00	30.18	30.39	30.58	34.32	34.44	34.52	31.22	31.24
1.416	1.575	1.612	1.723	1.818	1.888	1.893	1.936	1.963	1.979	1.988
3.994	4.185	4.234	4.415	4.624	4.853	4.876	5.110	5.353	5.595	5.838

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.792	1.787	1.772	1.769	1.766	1.763	1.790	1.789	1.787	1.785	1.788
31.25	31.26	41.26	41.24	41.22	41.19	31.24	31.24	31.24	31.25	31.28
1.993	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000	2.000
6.085	6.334	6.618	6.867	7.117	7.366	7.584	7.834	8.084	8.333	8.584

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1
1.786	1.784	1.781	1.769	1.765	1.761	
31.31	31.37	31.49	38.37	38.80	39.61	
2.000	2.000	2.000	2.000	2.000	2.000	
8.834	9.085	9.335	9.614	9.866	10.119	

68 DECYLSULFONIC ACID C10H2203S 222.30

-1	26.9	1.000					pHL	3.00	3.25	3.50
							RE	3.074	3.070	3.067
							t	32.83	29.17	26.85
							Z	0.996	0.998	0.998
							pHS	3.377	3.577	3.778

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.065	3.063	3.084	3.083	3.080	3.077	3.071	3.068	3.065	3.086	3.085
25.33	24.39	21.26	20.77	20.46	20.28	23.54	23.44	23.38	20.40	20.38
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.995	4.227	4.232	4.454	4.691	4.936	4.968	5.214	5.463	5.688	5.936

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.082	3.079	3.062	3.061	3.058	3.055	3.087	3.085	3.082	3.079	3.084
20.37	20.36	29.07	29.06	29.06	29.05	20.32	20.33	20.34	20.35	20.38
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.185	6.435	6.752	7.002	7.252	7.502	7.686	7.936	8.186	8.436	8.688

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12
3.081	3.078	3.073	3.060	3.054	3.045	
20.44	20.53	20.71	27.05	27.88	29.58	
1.000	1.000	1.000	1.000	1.000	1.000	
8.939	9.190	9.443	9.759	10.018	10.284	

69 DIBROMOFLUOROACETIC ACID C2HBr2FO2 235.84

-1	38.6	1.000					pHL	3.00	3.25	3.50
							RE	2.109	2.105	2.102
							t	25.94	23.13	21.40
							Z	0.995	0.997	0.998
							pHS	3.244	3.456	3.671

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.100	2.099	2.107	2.106	2.105	2.103	2.102	2.100	2.099	2.107	2.106
20.32	19.67	17.53	17.18	16.97	16.85	19.08	19.01	18.97	16.92	16.91
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.897	4.135	4.139	4.370	4.611	4.858	4.879	5.127	5.376	5.609	5.858

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.105	2.104	2.098	2.098	2.097	2.095	2.107	2.107	2.106	2.104	2.106
16.91	16.90	22.87	22.86	22.86	22.86	16.87	16.87	16.88	16.89	16.90
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.108	6.358	6.652	6.902	7.152	7.401	7.608	7.858	8.108	8.358	8.609

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12
2.105	2.104	2.102	2.098	2.095	2.093	
16.93	16.97	17.06	21.22	21.56	22.18	
1.000	1.000	1.000	1.000	1.000	1.000	
8.859	9.110	9.361	9.650	9.903	10.159	

70 2.3-DIBROMOPROPIONIC ACID C3H4Br2O2

-1 32.3 2.201 231.87

pHL	3.00	3.25	3.50
RE	2.688	2.630	2.593
t	28.66	25.68	23.78
Z	0.938	0.960	0.974
pHS	3.347	3.540	3.737

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.567	2.549	2.563	2.553	2.546	2.540	2.537	2.533	2.530	2.543	2.542
22.53	21.76	19.17	18.77	18.51	18.37	21.06	20.98	20.93	18.46	18.45
0.984	0.991	0.991	0.994	0.997	0.998	0.998	0.999	0.999	1.000	1.000
3.952	4.183	4.191	4.413	4.651	4.895	4.922	5.168	5.417	5.646	5.895
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.540	2.537	2.528	2.526	2.525	2.522	2.543	2.541	2.540	2.537	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.144	6.394	6.700	6.949	7.199	7.449	7.644	7.894	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

71 DICHLOROACETIC ACID (S) C2H2Cl2O2

-1 39.7 1.257 128.94

pHL	3.00	3.25	3.50
RE	2.057	2.050	2.045
t	25.48	22.74	21.06
Z	0.991	0.994	0.996
pHS	3.237	3.449	3.664

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.042	2.039	2.047	2.046	2.044	2.043	2.041	2.040	2.038	2.046	2.045
20.01	19.37	17.30	16.96	16.75	16.63	18.80	18.74	18.70	16.71	16.70
0.998	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.891	4.129	4.133	4.364	4.606	4.853	4.873	5.121	5.370	5.604	5.853
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.044	2.043	2.038	2.037	2.036	2.035	2.046	2.046	2.044	2.043	2.045
16.69	16.69	22.48	22.48	22.47	22.47	16.65	16.66	16.66	16.67	16.68
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.102	6.352	6.645	6.895	7.145	7.394	7.602	7.852	8.102	8.352	8.604
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
2.044	2.043	2.041	2.037	2.035	2.033					
16.71	16.75	16.83	20.87	21.18	21.76					
1.000	1.000	1.000	1.000	1.000	1.000					
8.854	9.104	9.355	9.643	9.896	10.151					

72 DICHLOROFLUOROACETIC ACID C2HCl2FO2

-1 36.5 1.000 146.93

pHL	3.00	3.25	3.50
RE	2.235	2.231	2.228
t	26.84	23.91	22.11
Z	0.995	0.997	0.998
pHS	3.264	3.474	3.686

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.226	2.225	2.234	2.233	2.232	2.230	2.228	2.227	2.225	2.235	2.234
20.97	20.28	18.02	17.64	17.42	17.29	19.66	19.59	19.55	17.37	17.36
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.911	4.148	4.152	4.382	4.623	4.869	4.892	5.139	5.388	5.620	5.869
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.233	2.231	2.224	2.224	2.222	2.221	2.235	2.234	2.233	2.231	2.234
17.35	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.119	6.368	6.666	6.916	7.166	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

73 2.4-DICHLOROPHENOL C6H4Cl2O

-1	31.3	7.699	163.00					pHL	3.00	3.25	3.50			
								RE	□□□□□	□□□□□	□□□□□			
								t	24.84	23.72	22.95			
								Z	0.008	0.010	0.012			
								pHS	5.628	5.715	5.794			
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75				
□□□□□	□□□□□	91.443	80.177	67.993	55.733	46.287	38.990	31.774	15.933	14.509				
22.34	21.87	18.94	18.84	18.75	18.67	21.26	21.23	21.21	18.78	18.77				
0.015	0.019	0.027	0.030	0.036	0.044	0.053	0.063	0.077	0.156	0.171				
5.878	5.972	6.127	6.186	6.259	6.349	6.435	6.513	6.609	6.949	6.997				
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50				
12.756	10.843	6.132	5.670	5.106	4.509	3.641	3.423	3.196	2.997	2.839				
18.77	18.77	25.98	25.99	26.00	26.03	18.72	18.72	18.73	18.74	18.76				
0.195	0.230	0.413	0.447	0.498	0.566	0.712	0.758	0.814	0.870	0.922				
7.066	7.155	7.521	7.582	7.669	7.786	8.058	8.162	8.306	8.488	8.735				
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3								
2.756	2.699	2.663	2.632	2.619	2.608									
18.80	18.87	18.99	24.29	24.85	25.93									
0.950	0.970	0.983	0.991	0.995	0.997									
8.943	9.173	9.415	9.717	9.969	10.228									

74 2.4-DICHLOROPHENOXYACETIC ACID C8H6Cl2O3

-1	25.0	1.000	221.00					pHL	3.00	3.25	3.50			
								RE	3.320	3.316	3.313			
								t	34.59	30.71	28.24			
								Z	0.996	0.998	0.999			
								pHS	3.405	3.602	3.801			
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75				
3.311	3.309	3.333	3.332	3.329	3.326	3.319	3.315	3.311	3.337	3.335				
26.62	25.60	22.22	21.69	21.36	21.16	24.69	24.58	24.51	21.30	21.27				
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000				
4.016	4.248	4.252	4.473	4.709	4.954	4.988	5.234	5.483	5.706	5.954				
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50				
3.332	3.328	3.308	3.306	3.303	3.299	3.337	3.335	3.332	3.328	3.334				
21.26	21.25	30.66	30.65	30.64	30.63	21.21	21.22	21.23	21.25	21.28				
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000				
6.203	6.453	6.775	7.024	7.274	7.524	7.704	7.954	8.204	8.454	8.707				
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12								
3.331	3.326	3.322	3.305	3.297	3.286									
21.35	21.46	21.66	28.60	29.63	31.79									
1.000	1.000	1.000	1.000	1.000	1.000									
8.958	9.209	9.462	9.785	10.045	10.315									

75 DICHROMIC ACID H2Cr2O7

-1	58.9	0.745	218.00					pHL	3.00	3.25	3.50			
-2	82.1	6.723						RE	1.359	1.357	1.355			
								t	20.62	18.48	17.24			
								Z	0.996	0.998	1.000			
								pHS	3.097	3.330	3.564			
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75				
1.354	1.353	1.355	1.354	1.352	1.349	1.348	1.343	1.334	1.320	1.298				
16.51	16.11	14.74	14.53	14.46	14.49	15.94	16.10	16.41	15.65	16.49				
1.001	1.002	1.002	1.005	1.009	1.015	1.016	1.028	1.048	1.089	1.146				
3.803	4.048	4.051	4.293	4.540	4.789	4.799	5.048	5.299	5.576	5.821				
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50				
1.266	1.227	1.166	1.133	1.103	1.079	1.070	1.017	1.054	1.051	1.049				
17.69	19.20	26.43	27.92	29.25	30.28	25.29	14.52	25.89	26.03	26.11				
1.232	1.347	1.528	1.643	1.750	1.838	1.904	1.006	1.966	1.980	1.989				
6.064	6.305	6.624	6.826	7.046	7.280	7.536	4.350	8.015	8.263	8.513				
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10								
1.048	1.047	1.046	1.042	1.041	1.040									
26.17	26.23	26.29	30.26	30.43	30.72									
1.994	1.996	1.998	1.999	1.999	2.000									
8.762	9.011	9.261	9.513	9.763	10.013									

76 DIETHYLACETIC ACID C6H12O2 160.17

-1 30.3 4.734

pHL	3.00	3.25	3.50
RE	11.668	9.780	8.360
t	26.19	24.74	23.75
Z	0.221	0.265	0.311
pHS	4.169	4.271	4.367

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.122	6.016	5.240	4.731	4.223	3.766	3.628	3.335	3.104	2.938	2.859
22.99	22.43	19.42	19.25	19.09	18.98	21.81	21.75	21.71	19.09	19.08
0.366	0.435	0.505	0.561	0.630	0.710	0.737	0.804	0.865	0.922	0.949
4.472	4.596	4.715	4.811	4.935	5.090	5.149	5.313	5.508	5.773	5.962
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.801	2.763	2.726	2.715	2.707	2.701	2.723	2.721	2.718	2.715	2.719
19.07	19.06	26.75	26.74	26.74	26.73	19.03	19.03	19.04	19.05	19.07
0.968	0.981	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.183	6.419	6.733	6.973	7.220	7.468	7.660	7.909	8.158	8.408	8.660
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.717	2.714	2.710	2.701	2.697	2.691					
19.12	19.19	19.32	24.83	25.43	26.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.911	9.162	9.413	9.720	9.976	10.238					

77 DIETHYLMALONIC ACID C7H12O4 116.16

-1 25.0 2.211

-2 49.5 7.290

pHL	3.00	3.25	3.50
RE	3.483	3.421	3.380
t	34.27	30.58	28.20
Z	0.948	0.966	0.978
pHS	3.435	3.623	3.814

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.351	3.330	3.354	3.341	3.328	3.314	3.305	3.285	3.256	3.239	3.169
26.62	25.62	22.23	21.72	21.42	21.27	24.81	24.79	24.89	21.95	22.37
0.987	0.993	0.993	0.997	1.000	1.004	1.005	1.010	1.019	1.034	1.059
4.024	4.251	4.260	4.477	4.712	4.955	4.991	5.236	5.483	5.734	5.978
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.062	2.912	2.576	2.413	2.250	2.105	2.010	1.941	1.888	1.852	1.835
23.04	24.00	35.80	36.93	38.06	39.06	30.02	30.48	30.83	31.06	31.23
1.100	1.162	1.325	1.425	1.539	1.657	1.774	1.846	1.902	1.941	1.966
6.221	6.461	6.855	7.037	7.232	7.440	7.685	7.885	8.109	8.347	8.597
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
1.822	1.812	1.806	1.791	1.786	1.781					
31.34	31.45	31.59	38.57	39.02	39.85					
1.980	1.989	1.994	1.997	1.998	1.999					
8.841	9.089	9.338	9.617	9.869	10.122					

78 DIFLUOROACETIC ACID C2H2F2O2 96.03

-1 40.6 1.000

pHL	3.00	3.25	3.50
RE	2.002	1.997	1.995
t	25.17	22.45	20.80
Z	0.995	0.997	0.998
pHS	3.226	3.440	3.657

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.993	1.991	1.998	1.998	1.996	1.995	1.994	1.992	1.991	1.998	1.998
19.76	19.14	17.12	16.78	16.58	16.47	18.59	18.52	18.49	16.54	16.53
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.885	4.123	4.127	4.359	4.602	4.848	4.868	5.116	5.365	5.600	5.849
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.997	1.996	1.991	1.990	1.989	1.988	1.999	1.998	1.997	1.996	1.998
16.52	16.52	22.18	22.18	22.17	22.17	16.49	16.49	16.50	16.51	16.52
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.098	6.348	6.639	6.889	7.139	7.389	7.598	7.848	8.098	8.348	8.599
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.997	1.995	1.994	1.990	1.988	1.986					
16.54	16.58	16.66	20.60	20.89	21.44					
1.000	1.000	1.000	1.000	1.000	1.000					
8.850	9.100	9.351	9.637	9.890	10.145					

79 2.4-DIHYDROXYBENZOIC ACID C7H604

-1 32.0 3.395 154.12

pHL	3.00	3.25	3.50
RE	3.987	3.585	3.288
t	27.09	24.99	23.57
Z	0.630	0.703	0.768
pHS	3.597	3.738	3.883

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.052	2.870	2.853	2.754	2.679	2.629	2.621	2.592	2.574	2.580	2.573
22.55	21.85	19.15	18.83	18.60	18.45	21.17	21.09	21.04	18.55	18.54
0.830	0.884	0.895	0.928	0.955	0.973	0.975	0.985	0.991	0.995	0.997
4.049	4.243	4.289	4.470	4.681	4.911	4.943	5.179	5.423	5.656	5.900
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.569	2.565	2.553	2.552	2.550	2.547	2.568	2.567	2.565	2.563	2.566
18.53	18.52	25.78	25.78	25.77	25.77	18.49	18.49	18.50	18.51	18.53
0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.147	6.396	6.703	6.952	7.202	7.452	7.646	7.896	8.146	8.396	8.648
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
2.564	2.562	2.559	2.551	2.547	2.542					
18.57	18.64	18.76	23.92	24.44	25.46					
1.000	1.000	1.000	1.000	1.000	1.000					
8.898	9.149	9.401	9.704	9.959	10.219					

80 2.5-DIHYDROXYBENZOIC ACID C7H604

-1 34.4 2.975 154.12

pHL	3.00	3.25	3.50
RE	3.065	2.845	2.690
t	26.52	24.22	22.70
Z	0.766	0.826	0.875
pHS	3.456	3.618	3.786

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.574	2.492	2.496	2.451	2.419	2.399	2.395	2.383	2.375	2.383	2.380
21.65	20.96	18.50	18.16	17.93	17.79	20.31	20.24	20.19	17.88	17.87
0.916	0.947	0.950	0.968	0.981	0.989	0.990	0.994	0.997	0.998	0.999
3.976	4.190	4.217	4.421	4.648	4.887	4.914	5.157	5.403	5.636	5.882
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.378	2.375	2.367	2.366	2.364	2.362	2.379	2.378	2.376	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.131	6.381	6.682	6.932	7.182	7.432	7.631	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

81 2.6-DIHYDROXYBENZOIC ACID C7H604

-1 37.2 1.301 154.12

pHL	3.00	3.25	3.50
RE	2.202	2.194	2.189
t	26.50	23.63	21.86
Z	0.990	0.994	0.996
pHS	3.261	3.470	3.682

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.185	2.182	2.192	2.190	2.188	2.186	2.185	2.183	2.181	2.191	2.190
20.74	20.07	17.85	17.48	17.26	17.14	19.46	19.39	19.35	17.22	17.21
0.998	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.907	4.144	4.148	4.378	4.619	4.865	4.887	5.135	5.384	5.616	5.865
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.188	2.187	2.181	2.180	2.179	2.177	2.191	2.190	2.189	2.187	2.190
17.20	17.20	23.40	23.39	23.39	23.39	17.16	17.17	17.17	17.18	17.19
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.115	6.365	6.661	6.911	7.161	7.411	7.615	7.865	8.115	8.365	8.616
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.188	2.187	2.185	2.180	2.177	2.174					
17.22	17.27	17.36	21.71	22.07	22.75					
1.000	1.000	1.000	1.000	1.000	1.000					
8.867	9.117	9.368	9.660	9.914	10.170					

82 3.4-DIHYDROXYBENZOIC ACID C7H604

-1	34.4	4.509			154.12		pHL	3.00	3.25	3.50
							RE	8.509	7.179	6.180
							t	24.19	22.92	22.04
							Z	0.268	0.318	0.371
							pHS	4.051	4.156	4.255

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.312	4.540	4.039	3.681	3.329	3.021	2.944	2.749	2.603	2.508	2.459
21.36	20.85	18.21	18.05	17.91	17.80	20.28	20.23	20.19	17.88	17.87
0.433	0.508	0.577	0.634	0.703	0.778	0.798	0.856	0.906	0.946	0.966
4.366	4.496	4.613	4.717	4.851	5.017	5.071	5.248	5.455	5.716	5.919
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.424	2.402	2.380	2.373	2.368	2.364	2.381	2.379	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.979	0.988	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.147	6.388	6.693	6.936	7.184	7.432	7.632	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

83 3.5-DIHYDROXYBENZOIC ACID C7H604

-1	34.4	4.051			154.12		pHL	3.00	3.25	3.50
							RE	5.802	4.988	4.376
							t	24.71	23.23	22.22
							Z	0.397	0.463	0.529
							pHS	3.843	3.959	4.073

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.855	3.409	3.224	2.999	2.798	2.640	2.614	2.519	2.455	2.429	2.408
21.45	20.89	18.30	18.09	17.92	17.79	20.30	20.23	20.19	17.88	17.87
0.602	0.684	0.728	0.785	0.843	0.895	0.903	0.938	0.962	0.978	0.987
4.201	4.354	4.446	4.577	4.744	4.943	4.984	5.193	5.422	5.667	5.895
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.393	2.384	2.371	2.368	2.365	2.363	2.380	2.378	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.137	6.383	6.686	6.934	7.182	7.432	7.631	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

84 DIHYDROXYTARTARIC ACID C4H608

-1	32.0	1.947			182.09		pHL	3.00	3.25	3.50
-2	60.0	4.004					RE	2.262	2.111	1.967
							t	32.61	30.62	29.92
							Z	1.174	1.276	1.389
							pHS	3.310	3.507	3.702

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.832	1.713	1.706	1.627	1.567	1.525	1.519	1.492	1.476	1.478	1.472
29.90	30.22	27.50	27.84	28.15	28.38	31.45	31.60	31.70	28.99	29.02
1.514	1.641	1.663	1.760	1.842	1.902	1.905	1.943	1.967	1.981	1.989
3.906	4.122	4.162	4.363	4.584	4.819	4.835	5.073	5.317	5.563	5.807
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.468	1.465	1.455	1.454	1.452	1.449	1.467	1.466	1.465	1.464	1.466
29.04	29.05	37.26	37.25	37.24	37.22	29.03	29.03	29.04	29.04	29.06
1.994	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000	2.000
6.055	6.304	6.576	6.825	7.075	7.324	7.554	7.803	8.053	8.303	8.554
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
1.465	1.463	1.462	1.454	1.451	1.449					
29.09	29.13	29.22	34.82	35.11	35.64					
2.000	2.000	2.000	2.000	2.000	2.000					
8.804	9.054	9.304	9.572	9.823	10.075					

85 2,3-DIMETHYLBENZOIC ACID C9H1002

-1	27.1	3.738	150.18				pHL	3.00	3.25	3.50
							RE	5.679	5.001	4.491
							t	29.86	27.61	26.09
							Z	0.523	0.596	0.665
							pHS	3.751	3.878	4.007

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.067	3.722	3.657	3.471	3.319	3.212	3.193	3.130	3.090	3.091	3.077
24.97	24.19	20.94	20.60	20.35	20.19	23.42	23.32	23.27	20.31	20.29
0.737	0.808	0.829	0.875	0.917	0.948	0.952	0.971	0.983	0.990	0.994
4.155	4.330	4.390	4.550	4.743	4.963	5.002	5.230	5.470	5.700	5.940
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.067	3.060	3.041	3.038	3.035	3.032	3.063	3.061	3.058	3.055	3.060
20.28	20.28	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.186	6.434	6.752	7.000	7.250	7.500	7.684	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

86 2,4-DIMETHYLBENZOIC ACID C9H1002

-1	27.1	4.182	150.18				pHL	3.00	3.25	3.50
							RE	7.891	6.765	5.912
							t	29.08	27.14	25.82
							Z	0.372	0.436	0.500
							pHS	3.932	4.045	4.156

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.181	4.552	4.303	3.980	3.687	3.455	3.409	3.269	3.174	3.139	3.106
24.83	24.12	20.81	20.55	20.33	20.18	23.39	23.31	23.26	20.31	20.29
0.573	0.655	0.700	0.758	0.821	0.878	0.889	0.928	0.956	0.974	0.985
4.282	4.431	4.518	4.646	4.809	5.004	5.050	5.257	5.484	5.723	5.950
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.084	3.069	3.046	3.041	3.037	3.033	3.064	3.061	3.059	3.055	3.060
20.28	20.27	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.991	0.995	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.190	6.436	6.754	7.001	7.250	7.500	7.684	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

87 2,5-DIMETHYLBENZOIC ACID C9H1002

-1	27.1	3.977	150.18				pHL	3.00	3.25	3.50
							RE	6.727	5.832	5.156
							t	29.42	27.35	25.94
							Z	0.439	0.508	0.576
							pHS	3.845	3.965	4.083

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.583	4.100	3.956	3.702	3.482	3.317	3.287	3.189	3.125	3.111	3.089
24.90	24.15	20.87	20.57	20.34	20.18	23.41	23.32	23.27	20.31	20.29
0.651	0.731	0.764	0.818	0.872	0.916	0.923	0.952	0.972	0.983	0.990
4.219	4.379	4.454	4.596	4.774	4.981	5.024	5.242	5.476	5.710	5.944
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.074	3.064	3.043	3.039	3.036	3.032	3.063	3.061	3.058	3.055	3.060
20.28	20.28	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.994	0.997	0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.188	6.435	6.753	7.001	7.250	7.500	7.684	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

88 2.6-DIMETHYLBENZOIC ACID C9H1002

-1 27.1 3.246 150.18

pHL	3.00	3.25	3.50
RE	4.280	3.917	3.653
t	30.85	28.18	26.38
Z	0.701	0.768	0.825
pHS	3.585	3.734	3.888

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.446	3.292	3.295	3.210	3.147	3.106	3.097	3.073	3.057	3.072	3.066
25.10	24.24	21.06	20.65	20.36	20.19	23.43	23.33	23.27	20.31	20.29
0.877	0.919	0.925	0.950	0.969	0.982	0.983	0.990	0.994	0.997	0.998
4.064	4.267	4.299	4.490	4.709	4.944	4.979	5.218	5.464	5.691	5.936
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.061	3.056	3.040	3.037	3.035	3.031	3.063	3.061	3.058	3.055	3.060
20.28	20.28	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.184	6.434	6.751	7.000	7.250	7.499	7.684	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

89 3.4-DIMETHYLBENZOIC ACID C9H1002

-1 27.1 4.408 150.18

pHL	3.00	3.25	3.50
RE	9.540	8.094	6.999
t	28.76	26.94	25.70
Z	0.306	0.362	0.420
pHS	4.032	4.140	4.244

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.053	5.224	4.806	4.394	4.005	3.679	3.604	3.402	3.258	3.185	3.135
24.76	24.08	20.75	20.51	20.32	20.17	23.38	23.30	23.26	20.31	20.29
0.488	0.568	0.623	0.684	0.753	0.822	0.838	0.890	0.930	0.959	0.975
4.361	4.499	4.597	4.712	4.859	5.038	5.090	5.282	5.498	5.744	5.960
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.101	3.079	3.051	3.044	3.038	3.033	3.064	3.062	3.059	3.055	3.060
20.28	20.27	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.985	0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.195	6.439	6.757	7.002	7.251	7.500	7.685	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

90 3.5-DIMETHYLBENZOIC ACID C9H1002

-1 27.1 4.301 150.18

pHL	3.00	3.25	3.50
RE	8.706	7.420	6.448
t	28.91	27.03	25.76
Z	0.336	0.396	0.457
pHS	3.984	4.094	4.202

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.610	4.880	4.550	4.182	3.841	3.563	3.503	3.332	3.213	3.161	3.120
24.79	24.10	20.78	20.53	20.32	20.18	23.39	23.31	23.26	20.31	20.29
0.528	0.609	0.660	0.720	0.786	0.850	0.864	0.910	0.944	0.967	0.980
4.323	4.466	4.558	4.680	4.834	5.021	5.070	5.269	5.491	5.733	5.955
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.092	3.074	3.048	3.042	3.037	3.033	3.064	3.061	3.059	3.055	3.060
20.28	20.27	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.988	0.993	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.193	6.437	6.755	7.002	7.250	7.500	7.684	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

91 DIMETHYLMALONIC ACID C5H8O4

-1	25.5	3.166	132.12				pHL	3.00	3.25	3.50
-2	51.1	6.059					RE	4.339	4.000	3.750
							t	32.53	29.62	27.71
							Z	0.738	0.803	0.858
							pHS	3.577	3.729	3.888

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.551	3.392	3.394	3.284	3.170	3.039	3.007	2.845	2.653	2.388	2.234
26.40	25.62	22.26	22.04	22.13	22.58	26.19	27.03	28.17	26.80	27.78
0.909	0.953	0.960	0.994	1.032	1.079	1.089	1.156	1.246	1.412	1.519
4.069	4.275	4.309	4.505	4.726	4.960	5.005	5.235	5.465	5.779	5.962
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.090	1.971	1.850	1.804	1.771	1.748	1.764	1.756	1.750	1.746	1.748
28.70	29.46	39.86	40.17	40.37	40.48	30.84	30.89	30.92	30.94	30.97
1.634	1.742	1.854	1.905	1.942	1.966	1.980	1.988	1.993	1.996	1.998
6.162	6.378	6.687	6.896	7.127	7.368	7.590	7.834	8.081	8.330	8.581
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
1.745	1.743	1.740	1.728	1.724	1.720					
31.01	31.07	31.18	37.90	38.31	39.08					
1.999	1.999	2.000	2.000	2.000	2.000					
8.831	9.081	9.331	9.609	9.860	10.113					

92 2.6-DINITROBENZOIC ACID C7H4N2O6

-1	31.3	1.140	212.12				pHL	3.00	3.25	3.50
							RE	2.628	2.622	2.618
							t	29.60	26.34	24.30
							Z	0.994	0.996	0.998
							pHS	3.321	3.525	3.731

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.616	2.613	2.628	2.626	2.624	2.622	2.618	2.616	2.613	2.628	2.627
22.98	22.18	19.51	19.08	18.82	18.67	21.45	21.37	21.32	18.77	18.75
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.952	4.186	4.191	4.417	4.656	4.901	4.929	5.175	5.424	5.653	5.901
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.625	2.623	2.612	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.400	6.708	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

93 3.5-DINITROBENZOIC ACID C7H4N2O6

-1	29.3	2.824	212.12				pHL	3.00	3.25	3.50
							RE	3.373	3.187	3.058
							t	29.90	27.07	25.19
							Z	0.824	0.874	0.912
							pHS	3.462	3.631	3.806

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.963	2.897	2.910	2.873	2.847	2.830	2.825	2.814	2.807	2.822	2.819
23.91	23.08	20.19	19.77	19.50	19.33	22.32	22.23	22.17	19.45	19.43
0.942	0.964	0.966	0.979	0.987	0.993	0.993	0.996	0.998	0.999	0.999
4.003	4.222	4.240	4.449	4.679	4.920	4.950	5.194	5.442	5.670	5.917
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.816	2.813	2.800	2.798	2.796	2.793	2.819	2.818	2.815	2.813	2.817
19.42	19.41	27.38	27.37	27.36	27.35	19.37	19.38	19.39	19.40	19.43
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.166	6.415	6.727	6.977	7.227	7.477	7.666	7.916	8.166	8.416	8.668
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.815	2.811	2.808	2.797	2.793	2.786					
19.47	19.55	19.69	25.42	26.08	27.39					
1.000	1.000	1.000	1.000	1.000	1.000					
8.919	9.169	9.421	9.731	9.988	10.250					

94 2.3-DINITROPHENOL C6H4N2O5
-1 31.3 4.018 184.11

pHL	3.00	3.25	3.50
RE	6.137	5.293	4.658
t	26.43	24.73	23.58
Z	0.414	0.481	0.549
pHS	3.842	3.959	4.075

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.118	3.658	3.490	3.254	3.046	2.886	2.859	2.763	2.699	2.678	2.656
22.71	22.08	19.24	18.99	18.80	18.66	21.43	21.36	21.31	18.77	18.75
0.623	0.704	0.743	0.799	0.855	0.904	0.912	0.944	0.967	0.981	0.988
4.206	4.362	4.446	4.583	4.754	4.956	4.998	5.211	5.442	5.682	5.913
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.642	2.632	2.617	2.614	2.611	2.608	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.156	6.403	6.711	6.959	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

95 2.4-DINITROPHENOL C6H4N2O5
-1 31.3 4.110 184.11

pHL	3.00	3.25	3.50
RE	6.592	5.658	4.955
t	26.29	24.65	23.53
Z	0.384	0.449	0.515
pHS	3.881	3.996	4.108

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.354	3.837	3.624	3.363	3.127	2.941	2.907	2.795	2.719	2.689	2.663
22.68	22.07	19.22	18.98	18.80	18.66	21.43	21.36	21.31	18.77	18.75
0.588	0.670	0.715	0.772	0.832	0.887	0.896	0.933	0.959	0.976	0.986
4.235	4.386	4.476	4.606	4.770	4.967	5.010	5.218	5.446	5.689	5.916
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.646	2.634	2.618	2.614	2.611	2.608	2.629	2.628	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.992	0.995	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.157	6.403	6.712	6.960	7.209	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

96 2.5-DINITROPHENOL C6H4N2O5
-1 31.3 5.216 184.11

pHL	3.00	3.25	3.50
RE	18.229	15.122	12.792
t	25.28	24.01	23.14
Z	0.136	0.164	0.194
pHS	4.397	4.493	4.581

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
10.752	8.904	7.235	6.453	5.638	4.860	4.523	4.022	3.581	3.123	2.980
22.47	21.95	19.02	18.88	18.76	18.66	21.36	21.32	21.29	18.76	18.75
0.232	0.281	0.350	0.393	0.451	0.526	0.566	0.639	0.720	0.835	0.876
4.677	4.787	4.923	5.002	5.104	5.232	5.302	5.433	5.594	5.885	6.030
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.854	2.762	2.679	2.651	2.632	2.620	2.637	2.632	2.628	2.624	2.628
18.74	18.74	26.16	26.16	26.15	26.15	18.70	18.71	18.71	18.73	18.75
0.916	0.947	0.974	0.984	0.991	0.995	0.997	0.998	0.999	0.999	1.000
6.217	6.434	6.752	6.976	7.215	7.461	7.656	7.903	8.152	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.625	2.622	2.619	2.611	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.904	9.154	9.406	9.710	9.966	10.226					

97 2.6-DINITROPHENOL C6H4N2O5

-1	31.3	3.706	184.11				pHL	3.00	3.25	3.50
							RE	4.911	4.317	3.873
							t	26.94	25.03	23.74
							Z	0.521	0.594	0.664
							pHS	3.714	3.842	3.971
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.505	3.206	3.140	2.980	2.850	2.758	2.744	2.690	2.656	2.653	2.641
22.79	22.11	19.31	19.02	18.81	18.66	21.44	21.36	21.31	18.77	18.75
0.736	0.807	0.830	0.876	0.917	0.948	0.952	0.971	0.983	0.990	0.994
4.119	4.294	4.359	4.518	4.711	4.930	4.966	5.194	5.433	5.668	5.907
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.633	2.627	2.614	2.612	2.610	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.153	6.402	6.710	6.959	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

98 3.4-DINITROPHENOL C6H4N2O5

-1	31.3	5.424	184.11				pHL	3.00	3.25	3.50
							RE	22.598	18.690	15.762
							t	25.19	23.95	23.10
							Z	0.109	0.132	0.157
							pHS	4.498	4.592	4.679
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
13.196	10.865	8.613	7.652	6.642	5.664	5.187	4.560	3.991	3.316	3.139
22.44	21.94	19.00	18.87	18.75	18.66	21.35	21.31	21.28	18.76	18.75
0.188	0.229	0.292	0.330	0.381	0.449	0.491	0.561	0.643	0.784	0.830
4.772	4.879	5.018	5.093	5.189	5.308	5.382	5.501	5.649	5.950	6.078
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.971	2.838	2.715	2.674	2.646	2.628	2.642	2.635	2.630	2.626	2.628
18.75	18.74	26.16	26.16	26.15	26.15	18.70	18.71	18.71	18.73	18.75
0.879	0.921	0.960	0.975	0.985	0.992	0.995	0.997	0.998	0.999	0.999
6.247	6.451	6.774	6.986	7.220	7.463	7.660	7.904	8.152	8.401	8.654
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.625	2.623	2.619	2.611	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.904	9.154	9.406	9.710	9.966	10.226					

99 3.5-DINITROPHENOL C6H4N2O5

-1	31.3	6.699	184.11				pHL	3.00	3.25	3.50
							RE	91.107	74.708	62.465
							t	24.90	23.76	22.97
							Z	0.027	0.032	0.039
							pHS	5.129	5.218	5.298
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
51.713	41.886	30.334	26.656	22.695	18.729	15.913	13.504	11.147	6.575	6.033
22.35	21.88	18.94	18.84	18.75	18.66	21.28	21.25	21.23	18.76	18.76
0.047	0.058	0.081	0.092	0.108	0.132	0.156	0.184	0.223	0.386	0.421
5.383	5.480	5.632	5.693	5.770	5.865	5.949	6.035	6.139	6.472	6.536
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
5.390	4.722	3.536	3.333	3.123	2.941	2.826	2.755	2.702	2.667	2.652
18.75	18.75	26.08	26.10	26.11	26.12	18.71	18.71	18.72	18.73	18.75
0.473	0.542	0.729	0.775	0.829	0.882	0.927	0.952	0.970	0.983	0.990
6.625	6.743	7.098	7.204	7.351	7.537	7.766	7.955	8.175	8.412	8.663
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.639	2.630	2.624	2.613	2.608	2.602					
18.79	18.86	18.98	24.28	24.83	25.92					
0.994	0.997	0.998	0.999	1.000	1.000					
8.908	9.156	9.407	9.711	9.966	10.227					

100 DIPHENYLACETIC ACID C14H12O2

-1	26.2	3.939	212.20

pHL	3.00	3.25	3.50
RE	6.729	5.853	5.190
t	30.24	28.06	26.57
Z	0.455	0.525	0.594
pHS	3.835	3.956	4.076

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.629	4.160	4.034	3.784	3.571	3.413	3.384	3.290	3.230	3.221	3.199
25.47	24.69	21.31	20.99	20.74	20.58	23.92	23.83	23.77	20.71	20.69
0.668	0.747	0.777	0.830	0.881	0.923	0.930	0.957	0.974	0.985	0.991
4.214	4.378	4.448	4.594	4.775	4.985	5.027	5.248	5.483	5.716	5.951

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.185	3.175	3.153	3.149	3.145	3.141	3.175	3.173	3.170	3.167	3.172
20.68	20.67	29.63	29.62	29.61	29.60	20.64	20.64	20.65	20.66	20.70
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.196	6.443	6.763	7.011	7.260	7.510	7.692	7.942	8.192	8.442	8.695

8.75	9.00	9.25	9.50	9.75	10.00
3.169	3.165	3.160	3.145	3.139	3.130
20.76	20.86	21.04	27.59	28.49	30.34
1.000	1.000	1.000	1.000	1.000	1.000
8.946	9.197	9.449	9.769	10.027	10.295

(Ref.) : 2 , 7

101 DIPROPYLMALONIC ACID C9H16O4

-1	23.0	2.067	188.22
-2	46.0	7.510	

pHL	3.00	3.25	3.50
RE	3.743	3.697	3.666
t	36.55	32.53	29.94
Z	0.964	0.976	0.985
pHS	3.458	3.646	3.837

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.645	3.630	3.658	3.648	3.638	3.626	3.616	3.601	3.578	3.579	3.526
28.21	27.12	23.42	22.86	22.51	22.33	26.19	26.13	26.16	22.82	23.09
0.991	0.995	0.995	0.998	1.000	1.003	1.003	1.006	1.012	1.021	1.037
4.047	4.274	4.282	4.498	4.733	4.976	5.013	5.259	5.506	5.745	5.991

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.442	3.316	2.992	2.803	2.605	2.417	2.275	2.175	2.095	2.038	2.007
23.55	24.27	36.53	37.70	38.92	40.09	30.52	31.12	31.59	31.93	32.18
1.064	1.108	1.231	1.322	1.432	1.554	1.693	1.779	1.854	1.909	1.947
6.237	6.481	6.879	7.073	7.272	7.480	7.728	7.918	8.134	8.367	8.617

8.75	9.00	9.25	9.50	9.75	10.00
1.985	1.970	1.960	1.941	1.934	1.928
32.34	32.48	32.66	40.26	40.79	41.79
1.969	1.982	1.990	1.995	1.997	1.998
8.858	9.104	9.353	9.636	9.888	10.142

(Ref.) : 12 , 7

102 DITHIONIC ACID H2S2O6

-1	48.2	0.200	162.13
-2	96.4	3.400	

pHL	3.00	3.25	3.50
RE	1.208	1.114	1.039
t	28.62	27.30	26.79
Z	1.421	1.550	1.671
pHS	3.118	3.340	3.557

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
0.983	0.944	0.943	0.920	0.904	0.895	0.894	0.888	0.885	0.885	0.884
26.62	26.60	24.87	24.88	24.91	24.93	26.76	26.78	26.79	25.11	25.11
1.775	1.855	1.862	1.914	1.948	1.970	1.970	1.983	1.990	1.995	1.997
3.780	4.013	4.036	4.264	4.503	4.748	4.748	4.994	5.242	5.496	5.744

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
0.884	0.883	0.880	0.880	0.879	0.879	0.883	0.883	0.883	0.883	0.883
25.12	25.12	30.06	30.06	30.05	30.05	25.09	25.09	25.10	25.11	25.11
1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
5.994	6.243	6.487	6.736	6.986	7.236	7.493	7.743	7.993	8.243	8.493

8.75	9.00	9.25	9.50	9.75	10.00
0.883	0.883	0.883	0.880	0.880	0.879
25.12	25.15	25.19	28.52	28.64	28.86
2.000	2.000	2.000	2.000	2.000	2.000
8.743	8.993	9.243	9.487	9.737	9.987

(Ref.) : 2 , 8

103 DITHIONOUS ACID H2S2O4

-1	34.5	0.300	130.13				pHL	3.00	3.25	3.50
-2	68.9	2.500					RE	1.349	1.313	1.290
							t	38.20	34.76	32.73
							Z	1.852	1.906	1.943
							pHS	3.110	3.334	3.563

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.276	1.267	1.274	1.269	1.265	1.263	1.260	1.258	1.256	1.263	1.263
31.53	30.83	28.34	27.95	27.72	27.60	30.24	30.17	30.13	27.71	27.70
1.966	1.980	1.981	1.989	1.994	1.996	1.996	1.998	1.999	1.999	2.000
3.800	4.043	4.048	4.289	4.535	4.784	4.790	5.039	5.288	5.534	5.783
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.262	1.261	1.254	1.254	1.252	1.251	1.263	1.263	1.262	1.261	1.262
27.69	27.69	34.75	34.74	34.73	34.72	27.65	27.65	27.65	27.66	27.67
2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
6.033	6.283	6.546	6.796	7.046	7.295	7.533	7.783	8.033	8.283	8.533
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 8				
1.262	1.261	1.260	1.254	1.253	1.251					
27.69	27.73	27.80	32.60	32.82	33.23					
2.000	2.000	2.000	2.000	2.000	2.000					
8.783	9.034	9.284	9.544	9.794	10.045					

104 DODECYLSULFONIC ACID C12H26O3S

-1	24.9	1.000	250.40				pHL	3.00	3.25	3.50
							RE	3.334	3.330	3.327
							t	34.69	30.80	28.32
							Z	0.996	0.998	0.999
							pHS	3.407	3.604	3.803

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.325	3.323	3.348	3.346	3.344	3.340	3.333	3.329	3.326	3.351	3.349
26.69	25.67	22.28	21.74	21.41	21.21	24.76	24.64	24.57	21.35	21.32
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
4.018	4.249	4.254	4.474	4.711	4.955	4.989	5.235	5.484	5.707	5.955
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.346	3.342	3.322	3.320	3.317	3.313	3.352	3.349	3.346	3.343	3.349
21.31	21.30	30.75	30.74	30.73	30.72	21.26	21.27	21.28	21.30	21.34
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.204	6.454	6.776	7.026	7.275	7.525	7.705	7.955	8.205	8.455	8.708
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
3.345	3.341	3.336	3.318	3.311	3.300					
21.40	21.51	21.72	28.69	29.73	31.93					
1.000	1.000	1.000	1.000	1.000	1.000					
8.959	9.210	9.463	9.787	10.047	10.317					

105 ENANTHYLIC ACID C7H14O2

-1	28.4	4.893	130.19				pHL	3.00	3.25	3.50
							RE	14.349	11.979	10.194
							t	27.30	25.76	24.71
							Z	0.192	0.230	0.271
							pHS	4.251	4.351	4.444

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
8.638	7.241	6.209	5.574	4.933	4.346	4.147	3.769	3.462	3.219	3.114
23.91	23.31	20.09	19.92	19.76	19.64	22.66	22.61	22.57	19.77	19.76
0.321	0.385	0.454	0.507	0.575	0.656	0.688	0.759	0.829	0.901	0.932
4.547	4.667	4.787	4.879	4.996	5.142	5.206	5.360	5.545	5.815	5.993
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.033	2.979	2.927	2.911	2.900	2.892	2.918	2.915	2.911	2.908	2.912
19.75	19.75	27.97	27.97	27.96	27.95	19.71	19.71	19.72	19.74	19.76
0.957	0.974	0.988	0.993	0.996	0.998	0.998	0.999	1.000	1.000	1.000
6.206	6.438	6.756	6.994	7.239	7.487	7.675	7.924	8.173	8.423	8.676
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
2.909	2.906	2.902	2.890	2.885	2.878					
19.81	19.90	20.05	25.99	26.71	28.15					
1.000	1.000	1.000	1.000	1.000	1.000					
8.926	9.177	9.429	9.741	9.998	10.262					

106 o-ETHOXYBENZOIC ACID C9H1003
-1 26.6 4.208 166.18

pHL	3.00	3.25	3.50
RE	8.187	7.011	6.121
t	29.45	27.48	26.13
Z	0.365	0.428	0.492
pHS	3.946	4.058	4.169

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.357	4.697	4.433	4.095	3.787	3.542	3.493	3.344	3.243	3.205	3.170
25.13	24.41	21.03	20.76	20.55	20.39	23.67	23.59	23.54	20.53	20.51
0.565	0.647	0.692	0.751	0.815	0.873	0.885	0.925	0.954	0.973	0.984
4.294	4.442	4.529	4.656	4.818	5.011	5.058	5.264	5.490	5.729	5.955
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.147	3.131	3.106	3.101	3.097	3.092	3.125	3.123	3.120	3.116	3.122
20.50	20.49	29.31	29.30	29.29	29.28	20.45	20.46	20.47	20.48	20.52
0.991	0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.195	6.441	6.760	7.007	7.256	7.505	7.689	7.938	8.188	8.438	8.691
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 2				
3.118	3.115	3.110	3.096	3.090	3.081					
20.57	20.67	20.85	27.28	28.14	29.90					
1.000	1.000	1.000	1.000	1.000	1.000					
8.942	9.193	9.445	9.763	10.022	10.288					

107 p-ETHOXYBENZOIC ACID C9H1003
-1 26.6 4.796 166.18

pHL	3.00	3.25	3.50
RE	13.806	11.558	9.861
t	28.73	27.01	25.84
Z	0.214	0.256	0.301
pHS	4.212	4.314	4.410

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
8.384	7.064	6.179	5.560	4.945	4.393	4.221	3.867	3.588	3.391	3.294
24.95	24.30	20.87	20.67	20.50	20.37	23.61	23.56	23.52	20.52	20.51
0.355	0.424	0.490	0.546	0.616	0.697	0.725	0.794	0.858	0.917	0.945
4.515	4.639	4.752	4.848	4.972	5.126	5.187	5.351	5.544	5.805	5.994
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.223	3.176	3.128	3.113	3.104	3.096	3.127	3.124	3.120	3.117	3.122
20.50	20.49	29.30	29.30	29.29	29.28	20.45	20.46	20.47	20.48	20.52
0.966	0.980	0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.214	6.450	6.771	7.011	7.258	7.506	7.690	7.939	8.189	8.439	8.691
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 2				
3.119	3.115	3.110	3.096	3.090	3.081					
20.57	20.67	20.85	27.28	28.14	29.90					
1.000	1.000	1.000	1.000	1.000	1.000					
8.942	9.193	9.445	9.763	10.022	10.288					

108 o-ETHYLBENZOIC ACID C9H1002
-1 26.5 3.793 150.18

pHL	3.00	3.25	3.50
RE	6.008	5.274	4.721
t	30.26	27.99	26.46
Z	0.505	0.577	0.647
pHS	3.776	3.901	4.028

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.258	3.879	3.801	3.596	3.428	3.307	3.286	3.215	3.170	3.169	3.153
25.33	24.53	21.21	20.87	20.61	20.44	23.75	23.66	23.60	20.58	20.56
0.720	0.793	0.816	0.864	0.908	0.942	0.947	0.968	0.981	0.989	0.994
4.173	4.345	4.407	4.563	4.754	4.971	5.012	5.238	5.477	5.707	5.946
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.142	3.134	3.114	3.111	3.108	3.104	3.137	3.135	3.132	3.129	3.134
20.54	20.54	29.39	29.38	29.37	29.36	20.50	20.50	20.51	20.53	20.56
0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.192	6.440	6.759	7.007	7.257	7.506	7.689	7.939	8.189	8.439	8.692
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.131	3.127	3.123	3.108	3.102	3.093					
20.62	20.72	20.90	27.35	28.22	30.01					
1.000	1.000	1.000	1.000	1.000	1.000					
8.943	9.194	9.446	9.765	10.023	10.290					

109 p-ETHYLBENZOIC ACID C9H1002 150.18

-1 26.5 4.353

pHL	3.00	3.25	3.50							
RE	9.270	7.886	6.837							
t	29.32	27.41	26.12							
Z	0.323	0.381	0.441							
pHS	4.010	4.119	4.225							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.933	5.142	4.772	4.374	4.004	3.698	3.630	3.441	3.308	3.247	3.201
25.14	24.44	21.04	20.79	20.58	20.43	23.72	23.64	23.59	20.57	20.55
0.510	0.591	0.644	0.704	0.772	0.838	0.853	0.901	0.938	0.964	0.978
4.345	4.486	4.580	4.698	4.850	5.033	5.084	5.280	5.500	5.743	5.962
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.170	3.150	3.122	3.115	3.110	3.105	3.138	3.135	3.132	3.129	3.134
20.54	20.54	29.39	29.38	29.37	29.36	20.50	20.50	20.51	20.53	20.56
0.987	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.199	6.443	6.763	7.009	7.257	7.507	7.690	7.939	8.189	8.439	8.692
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.131	3.127	3.123	3.108	3.102	3.093					
20.62	20.72	20.90	27.35	28.22	30.01					
1.000	1.000	1.000	1.000	1.000	1.000					
8.943	9.194	9.446	9.765	10.023	10.290					

110 2-ETHYLBUTYRIC ACID C6H1206 180.16

-1 30.2 4.734

pHL	3.00	3.25	3.50							
RE	11.701	9.808	8.383							
t	26.25	24.80	23.80							
Z	0.222	0.265	0.311							
pHS	4.169	4.271	4.367							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.143	6.033	5.257	4.746	4.237	3.778	3.639	3.346	3.114	2.948	2.869
23.04	22.47	19.45	19.28	19.13	19.01	21.85	21.79	21.76	19.12	19.11
0.366	0.436	0.505	0.561	0.631	0.710	0.737	0.804	0.866	0.923	0.949
4.473	4.596	4.715	4.811	4.936	5.090	5.150	5.314	5.509	5.773	5.963
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.811	2.773	2.736	2.724	2.716	2.711	2.733	2.730	2.728	2.725	2.728
19.10	19.10	26.81	26.80	26.80	26.79	19.06	19.06	19.07	19.09	19.11
0.968	0.981	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.183	6.420	6.734	6.974	7.221	7.469	7.661	7.909	8.159	8.409	8.661
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
2.726	2.723	2.720	2.710	2.706	2.700					
19.15	19.23	19.36	24.89	25.49	26.69					
1.000	1.000	1.000	1.000	1.000	1.000					
8.912	9.162	9.414	9.721	9.977	10.239					

111 ETHYLFUMARIC ACID C6H804 144.13

-1 29.2 3.325

pHL	3.00	3.25	3.50							
RE	4.166	3.778	3.493							
t	29.05	26.66	25.05							
Z	0.665	0.735	0.797							
pHS	3.592	3.737	3.886							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.268	3.098	3.092	2.998	2.928	2.882	2.873	2.847	2.830	2.840	2.834
23.89	23.11	20.16	19.79	19.53	19.37	22.36	22.27	22.22	19.48	19.46
0.854	0.902	0.910	0.940	0.962	0.978	0.979	0.988	0.993	0.996	0.998
4.058	4.256	4.295	4.481	4.696	4.929	4.962	5.200	5.445	5.675	5.919
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.829	2.824	2.811	2.808	2.806	2.803	2.829	2.828	2.826	2.823	2.827
19.45	19.45	27.44	27.43	27.43	27.42	19.41	19.42	19.42	19.44	19.46
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.167	6.416	6.729	6.978	7.228	7.478	7.666	7.916	8.166	8.416	8.669
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.825	2.822	2.818	2.807	2.803	2.796					
19.51	19.59	19.73	25.48	26.15	27.47					
1.000	1.000	1.000	1.000	1.000	1.000					
8.919	9.170	9.422	9.732	9.989	10.252					

112 3-ETHYLGLUTARIC ACID C7H12O4 160.17

-1	25.0	4.287								
-2	50.0	5.329								

pHL	3.00	3.25	3.50							
RE	8.621	7.242	6.187							
t	31.56	29.74	28.64							
Z	0.371	0.443	0.522							
pHS	3.980	4.089	4.195							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.266	4.443	3.998	3.561	3.132	2.749	2.654	2.391	2.179	2.018	1.938
28.00	27.83	24.66	25.01	25.64	26.53	30.41	31.35	32.29	29.92	30.36
0.617	0.737	0.831	0.939	1.077	1.239	1.284	1.437	1.589	1.748	1.828
4.313	4.452	4.554	4.670	4.817	4.991	5.043	5.222	5.424	5.696	5.889
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.877	1.837	1.798	1.784	1.775	1.768	1.793	1.791	1.788	1.785	1.789
30.70	30.93	41.07	41.13	41.16	41.16	31.22	31.23	31.24	31.25	31.27
1.891	1.935	1.965	1.980	1.988	1.993	1.996	1.998	1.999	1.999	2.000
6.110	6.346	6.636	6.874	7.120	7.367	7.586	7.834	8.084	8.334	8.585
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
1.787	1.784	1.781	1.769	1.765	1.761					
31.31	31.37	31.49	38.37	38.80	39.61					
2.000	2.000	2.000	2.000	2.000	2.000					
8.835	9.085	9.335	9.614	9.866	10.119					

113 ETHYLMALEIC ACID C6H8O4 144.13

-1	29.2	2.959								

pHL	3.00	3.25	3.50							
RE	3.543	3.313	3.149							
t	29.75	27.02	25.21							
Z	0.786	0.843	0.888							
pHS	3.492	3.654	3.823							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.027	2.941	2.952	2.904	2.870	2.848	2.841	2.828	2.819	2.834	2.830
23.95	23.13	20.22	19.80	19.53	19.37	22.36	22.27	22.22	19.48	19.46
0.925	0.953	0.955	0.972	0.983	0.990	0.991	0.995	0.997	0.998	0.999
4.014	4.229	4.251	4.455	4.682	4.922	4.953	5.196	5.443	5.671	5.918
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.827	2.823	2.810	2.808	2.806	2.803	2.829	2.828	2.826	2.823	2.827
19.45	19.45	27.44	27.43	27.43	27.42	19.41	19.42	19.42	19.44	19.46
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.167	6.416	6.729	6.978	7.228	7.478	7.666	7.916	8.166	8.416	8.669
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.825	2.822	2.818	2.807	2.803	2.796					
19.51	19.59	19.73	25.48	26.15	27.47					
1.000	1.000	1.000	1.000	1.000	1.000					
8.919	9.170	9.422	9.732	9.989	10.252					

114 ETHYLMALONIC ACID C5H8O4 132.12

-1	25.5	2.988								
-2	51.0	5.833								

pHL	3.00	3.25	3.50							
RE	4.032	3.769	3.575							
t	32.91	29.86	27.87							
Z	0.797	0.854	0.903							
pHS	3.534	3.695	3.862							
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.418	3.285	3.291	3.182	3.054	2.896	2.857	2.670	2.465	2.225	2.096
26.57	25.87	22.53	22.43	22.72	23.42	27.11	28.17	29.43	27.90	28.72
0.946	0.987	0.993	1.029	1.075	1.138	1.153	1.241	1.353	1.530	1.634
4.051	4.264	4.296	4.499	4.723	4.956	5.003	5.227	5.451	5.754	5.936
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.982	1.894	1.811	1.779	1.756	1.741	1.761	1.756	1.752	1.748	1.751
29.45	30.02	40.22	40.42	40.54	40.60	30.91	30.94	30.96	30.97	31.00
1.737	1.825	1.903	1.940	1.964	1.979	1.988	1.993	1.996	1.998	1.999
6.140	6.363	6.663	6.884	7.121	7.366	7.586	7.832	8.081	8.330	8.581
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
1.749	1.746	1.743	1.732	1.728	1.724					
31.04	31.10	31.21	37.94	38.36	39.13					
1.999	2.000	2.000	2.000	2.000	2.000					
8.831	9.081	9.332	9.609	9.861	10.114					

115 ETHYLPROPYLMALONIC ACID C8H1404 174.20

-1	23.5	2.145						pHL	3.00	3.25	3.50
-2	47.0	7.430						RE	3.685	3.631	3.595
								t	35.92	32.01	29.48
								Z	0.957	0.971	0.982
								pHS	3.454	3.641	3.832

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.570	3.552	3.579	3.567	3.556	3.543	3.532	3.515	3.490	3.485	3.425
27.79	26.72	23.10	22.56	22.22	22.05	25.83	25.78	25.83	22.60	22.92
0.989	0.994	0.994	0.997	1.000	1.003	1.004	1.008	1.014	1.025	1.044
4.041	4.269	4.276	4.493	4.727	4.971	5.007	5.253	5.500	5.743	5.988
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.331	3.193	2.855	2.672	2.484	2.310	2.185	2.096	2.027	1.978	1.953
23.45	24.26	36.44	37.60	38.78	39.88	30.44	30.98	31.40	31.69	31.91
1.076	1.126	1.265	1.360	1.472	1.593	1.725	1.806	1.873	1.922	1.955
6.233	6.475	6.874	7.063	7.260	7.467	7.713	7.906	8.126	8.360	8.610
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
1.934	1.922	1.913	1.896	1.889	1.883					
32.05	32.17	32.34	39.75	40.26	41.20					
1.974	1.985	1.991	1.995	1.997	1.999					
8.852	9.099	9.348	9.631	9.882	10.136					

116 ETHYLSULFONIC ACID C2H6O3S 110.13

-1	41.0	-2.000						pHL	3.00	3.25	3.50
								RE	1.971	1.971	1.971
								t	25.06	22.34	20.69
								Z	1.000	1.000	1.000
								pHS	3.219	3.435	3.653

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.970	1.970	1.977	1.976	1.975	1.974	1.973	1.972	1.971	1.978	1.977
19.66	19.04	17.04	16.71	16.51	16.40	18.49	18.43	18.39	16.47	16.46
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.882	4.121	4.124	4.357	4.600	4.847	4.866	5.113	5.363	5.598	5.847
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.976	1.975	1.971	1.970	1.969	1.968	1.978	1.978	1.977	1.975	1.977
16.45	16.45	22.05	22.05	22.04	22.04	16.42	16.42	16.43	16.44	16.44
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.096	6.346	6.637	6.887	7.137	7.386	7.596	7.846	8.096	8.346	8.597
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.976	1.975	1.973	1.970	1.968	1.966					
16.47	16.51	16.59	20.48	20.77	21.31					
1.000	1.000	1.000	1.000	1.000	1.000					
8.848	9.098	9.349	9.634	9.887	10.142					

117 FLUOROACETIC ACID C2H3FO2 78.04

-1	46.0	2.584						pHL	3.00	3.25	3.50
								RE	2.051	1.946	1.875
								t	22.62	20.62	19.34
								Z	0.849	0.896	0.931
								pHS	3.296	3.481	3.672

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.826	1.793	1.797	1.779	1.767	1.760	1.759	1.754	1.751	1.755	1.754
18.49	17.96	16.17	15.89	15.72	15.62	17.48	17.42	17.39	15.68	15.67
0.956	0.974	0.975	0.985	0.991	0.995	0.995	0.997	0.998	0.999	0.999
3.882	4.110	4.128	4.348	4.585	4.829	4.846	5.092	5.340	5.579	5.827
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.753	1.752	1.749	1.748	1.748	1.747	1.754	1.753	1.753	1.752	1.753
15.67	15.66	20.63	20.63	20.63	20.63	15.63	15.64	15.64	15.65	15.66
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.076	6.326	6.609	6.859	7.109	7.359	7.576	7.826	8.076	8.326	8.577
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1				
1.752	1.751	1.750	1.748	1.747	1.745					
15.68	15.71	15.77	19.20	19.42	19.83					
1.000	1.000	1.000	1.000	1.000	1.000					
8.827	9.077	9.328	9.606	9.858	10.112					

118 m-FLUOROBENZOIC ACID C7H5FO2 140.11
-1 33.4 3.865

pHL	3.00	3.25	3.50
RE	5.181	4.502	3.993
t	25.48	23.83	22.71
Z	0.460	0.531	0.600
pHS	3.768	3.890	4.011

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.565	3.207	3.095	2.909	2.751	2.633	2.615	2.546	2.501	2.488	2.473
21.87	21.27	18.62	18.38	18.19	18.06	20.64	20.57	20.53	18.15	18.14
0.674	0.752	0.785	0.836	0.886	0.927	0.932	0.958	0.975	0.986	0.992
4.150	4.314	4.392	4.538	4.719	4.929	4.967	5.187	5.422	5.661	5.896
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.463	2.456	2.444	2.441	2.439	2.436	2.455	2.453	2.452	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.141	6.388	6.693	6.941	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

119 o-FLUOROBENZOIC ACID C7H5FO2 140.11
-1 33.4 3.267

pHL	3.00	3.25	3.50
RE	3.588	3.255	3.012
t	26.53	24.42	23.00
Z	0.672	0.742	0.804
pHS	3.546	3.693	3.845

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.821	2.679	2.671	2.593	2.536	2.498	2.492	2.470	2.456	2.463	2.458
21.99	21.31	18.75	18.42	18.19	18.06	20.65	20.58	20.53	18.15	18.14
0.860	0.907	0.915	0.943	0.965	0.979	0.980	0.989	0.993	0.996	0.998
4.019	4.220	4.260	4.448	4.665	4.899	4.928	5.167	5.412	5.645	5.890
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.454	2.451	2.441	2.440	2.438	2.436	2.454	2.453	2.451	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.138	6.387	6.691	6.940	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

120 p-FLUOROBENZOIC ACID C7H5FO2 140.11
-1 34.2 4.142

pHL	3.00	3.25	3.50
RE	6.264	5.362	4.684
t	24.69	23.24	22.26
Z	0.369	0.432	0.496
pHS	3.884	3.997	4.108

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.103	3.601	3.370	3.121	2.893	2.710	2.677	2.566	2.490	2.455	2.429
21.50	20.95	18.34	18.13	17.96	17.85	20.36	20.30	20.26	17.94	17.92
0.568	0.650	0.700	0.758	0.819	0.876	0.887	0.926	0.955	0.974	0.984
4.232	4.380	4.477	4.602	4.763	4.955	4.999	5.202	5.428	5.675	5.900
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.412	2.401	2.387	2.383	2.380	2.377	2.394	2.393	2.391	2.389	2.392
17.91	17.91	24.68	24.68	24.67	24.67	17.87	17.88	17.88	17.90	17.91
0.991	0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.139	6.385	6.689	6.935	7.184	7.434	7.632	7.882	8.132	8.382	8.634
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.391	2.389	2.386	2.380	2.377	2.372					
17.95	18.00	18.11	22.89	23.33	24.18					
1.000	1.000	1.000	1.000	1.000	1.000					
8.884	9.135	9.386	9.684	9.938	10.197					

121 FORMIC ACID (S) CH2O2 46.03

-1	56.6	3.752					pHL	3.00	3.25	3.50
							RE	2.988	2.593	2.300
							t	18.60	17.73	17.12
							Z	0.464	0.536	0.605
							pHS	3.659	3.782	3.904

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.055	1.850	1.766	1.666	1.579	1.514	1.508	1.469	1.445	1.432	1.424
16.66	16.32	14.77	14.63	14.52	14.45	15.93	15.90	15.87	14.49	14.48
0.679	0.756	0.795	0.844	0.891	0.930	0.934	0.959	0.976	0.986	0.992
4.042	4.205	4.301	4.445	4.626	4.836	4.863	5.080	5.315	5.569	5.803
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.419	1.416	1.413	1.412	1.411	1.410	1.413	1.413	1.413	1.412	1.413
14.48	14.48	18.48	18.48	18.48	18.48	14.45	14.45	14.46	14.46	14.47
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.047	6.295	6.566	6.814	7.063	7.313	7.543	7.793	8.043	8.293	8.544
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
1.413	1.412	1.412	1.411	1.410	1.409					
14.48	14.51	14.55	17.28	17.43	17.69					
1.000	1.000	1.000	1.000	1.000	1.000					
8.794	9.044	9.294	9.561	9.812	10.063					

122 FUMARIC ACID C4H4O4 116.07

-1	31.0	3.019					pHL	3.00	3.25	3.50
-2	61.2	4.384					RE	2.995	2.666	2.400
							t	30.64	28.88	28.13
							Z	0.886	1.002	1.122
							pHS	3.471	3.630	3.792

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.164	1.956	1.912	1.777	1.663	1.577	1.566	1.511	1.475	1.464	1.451
28.06	28.50	25.95	26.51	27.10	27.60	30.62	30.97	31.21	28.65	28.74
1.255	1.402	1.449	1.571	1.691	1.794	1.802	1.874	1.924	1.956	1.974
3.971	4.169	4.232	4.411	4.614	4.836	4.859	5.084	5.321	5.572	5.809
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.443	1.438	1.426	1.424	1.422	1.419	1.436	1.435	1.434	1.433	1.435
28.78	28.81	36.86	36.86	36.85	36.84	28.81	28.82	28.82	28.83	28.85
1.985	1.992	1.995	1.997	1.999	1.999	2.000	2.000	2.000	2.000	2.000
6.054	6.302	6.573	6.821	7.071	7.320	7.550	7.800	8.050	8.300	8.551
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
1.434	1.432	1.431	1.423	1.421	1.419					
28.87	28.92	29.00	34.48	34.76	35.27					
2.000	2.000	2.000	2.000	2.000	2.000					
8.801	9.051	9.301	9.568	9.819	10.070					

123 GALLIC ACID C7H6O5 170.12

-1	34.4	4.469					pHL	3.00	3.25	3.50
							RE	8.212	6.938	5.980
							t	24.23	22.94	22.05
							Z	0.278	0.330	0.384
							pHS	4.032	4.138	4.238

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.149	4.412	3.948	3.604	3.267	2.975	2.905	2.721	2.584	2.499	2.452
21.37	20.85	18.22	18.05	17.91	17.80	20.28	20.23	20.19	17.88	17.87
0.447	0.524	0.590	0.649	0.717	0.790	0.809	0.866	0.913	0.950	0.968
4.350	4.482	4.597	4.703	4.840	5.009	5.062	5.242	5.451	5.710	5.916
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.420	2.399	2.379	2.372	2.368	2.364	2.380	2.379	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.981	0.989	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.146	6.387	6.692	6.936	7.183	7.432	7.632	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

124 GLUCONIC ACID C6H1207

-1	27.2	3.662	196.16				pHL	3.00	3.25	3.50
							RE	5.387	4.769	4.306
							t	29.92	27.63	26.07
							Z	0.550	0.623	0.692
							pHS	3.722	3.852	3.984

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.924	3.617	3.569	3.402	3.268	3.175	3.159	3.105	3.071	3.075	3.062
24.93	24.14	20.92	20.57	20.31	20.14	23.36	23.27	23.21	20.27	20.25
0.762	0.830	0.847	0.890	0.928	0.956	0.959	0.975	0.986	0.992	0.995
4.137	4.317	4.372	4.537	4.735	4.958	4.996	5.226	5.467	5.697	5.938
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.054	3.047	3.029	3.026	3.023	3.020	3.051	3.049	3.047	3.043	3.048
20.24	20.23	28.84	28.84	28.83	28.82	20.20	20.20	20.21	20.22	20.25
0.997	0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.185	6.433	6.750	6.999	7.249	7.498	7.683	7.933	8.183	8.433	8.686
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
3.045	3.042	3.037	3.024	3.018	3.010					
20.31	20.40	20.57	26.83	27.63	29.28					
1.000	1.000	1.000	1.000	1.000	1.000					
8.936	9.188	9.440	9.756	10.014	10.279					

125 GLUCURONIC ACID C6H1007

-1	26.7	3.677	194.14				pHL	3.00	3.25	3.50
							RE	5.527	4.890	4.412
							t	30.31	27.98	26.40
							Z	0.546	0.619	0.689
							pHS	3.731	3.860	3.992

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.017	3.700	3.650	3.477	3.338	3.241	3.224	3.168	3.132	3.137	3.124
25.24	24.43	21.15	20.79	20.53	20.36	23.64	23.55	23.49	20.49	20.47
0.759	0.827	0.845	0.888	0.926	0.955	0.958	0.975	0.985	0.991	0.995
4.144	4.323	4.378	4.543	4.741	4.963	5.001	5.232	5.472	5.702	5.943
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.115	3.108	3.089	3.086	3.083	3.079	3.112	3.110	3.107	3.104	3.109
20.46	20.45	29.23	29.22	29.21	29.20	20.41	20.42	20.42	20.44	20.47
0.997	0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.189	6.438	6.756	7.005	7.254	7.504	7.688	7.938	8.187	8.438	8.690
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
3.106	3.102	3.098	3.084	3.078	3.069					
20.53	20.62	20.80	27.20	28.05	29.79					
1.000	1.000	1.000	1.000	1.000	1.000					
8.941	9.192	9.444	9.762	10.020	10.287					

126 GLUTACONIC ACID C5H604

-1	28.0	3.767	130.10				pHL	3.00	3.25	3.50
-2	56.0	5.077					RE	5.272	4.542	3.978
							t	29.98	28.17	27.13
							Z	0.546	0.637	0.731
							pHS	3.747	3.872	3.998

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.486	3.048	2.879	2.610	2.352	2.125	2.081	1.920	1.793	1.709	1.661
26.62	26.65	23.88	24.42	25.23	26.21	29.64	30.52	31.27	28.97	29.28
0.840	0.967	1.036	1.150	1.286	1.436	1.466	1.600	1.722	1.833	1.891
4.140	4.307	4.394	4.542	4.718	4.917	4.959	5.157	5.374	5.641	5.850
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.627	1.605	1.581	1.573	1.567	1.563	1.583	1.581	1.579	1.577	1.580
29.50	29.64	38.57	38.60	38.61	38.61	29.80	29.80	29.81	29.82	29.84
1.934	1.961	1.979	1.988	1.993	1.996	1.998	1.999	1.999	2.000	2.000
6.080	6.322	6.602	6.845	7.092	7.340	7.565	7.815	8.064	8.314	8.565
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 1				
1.578	1.577	1.575	1.565	1.563	1.560					
29.87	29.92	30.01	36.07	36.40	37.03					
2.000	2.000	2.000	2.000	2.000	2.000					
8.815	9.065	9.315	9.587	9.838	10.091					

127 GLUTAMIC ACID (S) C5H9N04 147.13

1	28.9	2.155					pHL	3.00	3.25	3.50
-1	-28.9	4.376					RE	8.843	7.502	6.489
-2	-49.6	9.960					t	27.92	26.10	24.85
							Z	0.309	0.366	0.424
							pHS	4.030	4.132	4.232

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.614	4.846	4.447	4.072	3.717	3.420	3.353	3.169	3.038	2.971	2.926
23.90	23.20	20.05	19.81	19.62	19.47	22.47	22.40	22.35	19.59	19.58
0.492	0.573	0.630	0.690	0.758	0.827	0.843	0.893	0.932	0.961	0.976
4.345	4.481	4.581	4.695	4.842	5.021	5.072	5.264	5.481	5.728	5.944
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.895	2.875	2.850	2.842	2.836	2.828	2.850	2.839	2.821	2.792	2.748
19.57	19.57	27.65	27.66	27.68	27.71	19.65	19.75	19.93	20.24	20.80
0.986	0.992	0.997	0.999	1.001	1.004	1.006	1.012	1.021	1.036	1.066
6.180	6.423	6.738	6.984	7.232	7.481	7.675	7.924	8.174	8.424	8.693
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 5				
2.675	2.571	2.438	2.249	2.116	2.001					
21.63	22.84	24.43	32.87	34.99	37.27					
1.111	1.180	1.278	1.432	1.562	1.688					
8.938	9.182	9.421	9.715	9.938	10.169					

128 GLUTARIC ACID C5H804 132.12

-1	26.6	4.343					pHL	3.00	3.25	3.50
-2	55.6	5.272					RE	8.432	7.032	5.967
							t	30.12	28.53	27.59
							Z	0.353	0.425	0.503
							pHS	3.994	4.102	4.205

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.037	4.205	3.699	3.275	2.858	2.486	2.392	2.144	1.946	1.793	1.722
27.07	26.96	24.09	24.45	25.04	25.85	29.39	30.20	30.99	28.81	29.18
0.598	0.720	0.828	0.939	1.081	1.248	1.297	1.452	1.605	1.764	1.840
4.319	4.453	4.563	4.673	4.813	4.981	5.033	5.205	5.404	5.679	5.871
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.670	1.635	1.602	1.591	1.583	1.577	1.596	1.594	1.592	1.590	1.593
29.46	29.65	38.68	38.73	38.75	38.75	29.88	29.89	29.89	29.90	29.92
1.900	1.940	1.968	1.981	1.989	1.994	1.996	1.998	1.999	1.999	2.000
6.091	6.327	6.611	6.849	7.095	7.342	7.567	7.816	8.066	8.315	8.566
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.591	1.589	1.587	1.578	1.575	1.572					
29.95	30.01	30.10	36.20	36.55	37.18					
2.000	2.000	2.000	2.000	2.000	2.000					
8.816	9.066	9.317	9.589	9.840	10.092					

129 GLYCERIC ACID C3H604 106.08

-1	36.4	3.737					pHL	3.00	3.25	3.50
							RE	4.395	3.843	3.430
							t	24.23	22.68	21.62
							Z	0.497	0.570	0.640
							pHS	3.703	3.830	3.956

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.087	2.806	2.727	2.580	2.458	2.370	2.359	2.307	2.274	2.266	2.255
20.83	20.26	17.85	17.62	17.43	17.31	19.68	19.62	19.58	17.40	17.38
0.714	0.787	0.815	0.863	0.907	0.941	0.945	0.967	0.980	0.989	0.993
4.100	4.271	4.345	4.499	4.687	4.903	4.937	5.161	5.399	5.639	5.877
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.247	2.242	2.233	2.231	2.229	2.227	2.242	2.241	2.239	2.238	2.240
17.38	17.37	23.72	23.71	23.71	23.71	17.34	17.34	17.35	17.36	17.37
0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.122	6.370	6.669	6.918	7.167	7.417	7.619	7.869	8.119	8.369	8.621
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
2.239	2.237	2.235	2.230	2.227	2.224					
17.40	17.46	17.55	22.00	22.38	23.10					
1.000	1.000	1.000	1.000	1.000	1.000					
8.871	9.122	9.373	9.666	9.920	10.177					

130 GLYCOLIC ACID C2H4O3

-1	42.4	3.886	76.05				pHL	3.00	3.25	3.50
							RE	4.264	3.687	3.256
							t	21.78	20.58	19.76
							Z	0.437	0.506	0.574
							pHS	3.747	3.867	3.985

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.892	2.585	2.463	2.309	2.175	2.072	2.059	1.998	1.958	1.940	1.927
19.13	18.67	16.59	16.41	16.26	16.16	18.18	18.12	18.09	16.23	16.22
0.649	0.728	0.768	0.821	0.873	0.917	0.923	0.951	0.971	0.983	0.990
4.119	4.278	4.370	4.509	4.684	4.890	4.924	5.139	5.372	5.620	5.852
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.918	1.913	1.906	1.904	1.903	1.901	1.910	1.909	1.908	1.907	1.909
16.21	16.21	21.62	21.61	21.61	21.61	16.18	16.18	16.19	16.20	16.20
0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.095	6.342	6.632	6.879	7.129	7.378	7.591	7.840	8.090	8.340	8.591
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.908	1.907	1.905	1.902	1.901	1.899					
16.23	16.27	16.34	20.09	20.36	20.85					
1.000	1.000	1.000	1.000	1.000	1.000					
8.841	9.092	9.343	9.626	9.878	10.133					

131 GLYOXYLIC ACID C2H4O4

-1	39.6	3.337	92.05				pHL	3.00	3.25	3.50
							RE	3.196	2.867	2.628
							t	23.57	21.89	20.75
							Z	0.631	0.705	0.771
							pHS	3.538	3.681	3.829

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.438	2.293	2.275	2.197	2.139	2.100	2.096	2.074	2.060	2.061	2.056
19.93	19.37	17.21	16.95	16.77	16.65	18.82	18.76	18.72	16.73	16.72
0.832	0.886	0.898	0.930	0.956	0.974	0.975	0.986	0.992	0.995	0.997
3.997	4.192	4.242	4.424	4.637	4.868	4.894	5.130	5.375	5.613	5.856
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.053	2.050	2.044	2.043	2.042	2.040	2.052	2.051	2.050	2.049	2.051
16.71	16.71	22.51	22.51	22.51	22.51	16.67	16.68	16.68	16.69	16.70
0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.104	6.353	6.646	6.896	7.145	7.395	7.603	7.853	8.103	8.353	8.604
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.050	2.048	2.046	2.042	2.040	2.038					
16.73	16.77	16.85	20.90	21.21	21.80					
1.000	1.000	1.000	1.000	1.000	1.000					
8.854	9.105	9.356	9.643	9.896	10.152					

132 HIPPURIC ACID C9H9NO3

-1	25.3	2.700	179.18				pHL	3.00	3.25	3.50
-2	55.1	7.271					RE	3.744	3.586	3.477
							t	33.47	30.10	27.88
							Z	0.868	0.907	0.937
							pHS	3.484	3.656	3.835

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.397	3.341	3.362	3.329	3.302	3.278	3.268	3.241	3.203	3.170	3.084
26.37	25.41	22.05	21.56	21.27	21.13	24.62	24.60	24.69	21.81	22.23
0.960	0.976	0.977	0.987	0.995	1.001	1.002	1.009	1.019	1.036	1.062
4.035	4.257	4.271	4.482	4.713	4.954	4.990	5.234	5.481	5.739	5.982
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.954	2.778	2.390	2.224	2.060	1.913	1.806	1.739	1.687	1.653	1.635
22.89	23.79	34.85	35.69	36.52	37.25	28.95	29.31	29.58	29.76	29.89
1.104	1.168	1.340	1.435	1.545	1.659	1.780	1.848	1.903	1.942	1.966
6.222	6.459	6.863	7.033	7.220	7.424	7.677	7.872	8.093	8.329	8.579
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
1.622	1.614	1.608	1.596	1.592	1.588					
29.98	30.07	30.19	36.36	36.72	37.37					
1.981	1.989	1.994	1.997	1.998	1.999					
8.823	9.070	9.319	9.592	9.843	10.095					

133 HYDROBROMIC ACID HBr

-1	81.0	-2.000	80.91				pHL	3.00	3.25	3.50
							RE	0.976	0.976	0.976
							t	17.88	16.11	15.11
							Z	1.000	1.000	1.000
							pHS	2.993	3.244	3.495

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976
14.56	14.25	13.27	13.09	12.99	12.94	13.97	13.94	13.93	12.97	12.96
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.746	3.996	3.996	4.247	4.497	4.747	4.747	4.997	5.247	5.497	5.747

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976	0.976
12.96	12.97	15.72	15.72	15.72	15.73	12.94	12.95	12.95	12.95	12.95
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
5.997	6.247	6.496	6.746	6.996	7.246	7.497	7.747	7.997	8.247	8.497

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12
0.976	0.976	0.976	0.976	0.976	0.976	
12.96	12.98	13.00	14.87	14.94	15.08	
1.000	1.000	1.000	1.000	1.000	1.000	
8.747	8.997	9.247	9.496	9.746	9.996	

134 HYDROCHLORIC ACID HCl

-1	79.1	-2.000	36.46				pHL	3.00	3.25	3.50
							RE	1.000	1.000	1.000
							t	18.06	16.26	15.25
							Z	1.000	1.000	1.000
							pHS	3.000	3.250	3.500

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
14.68	14.36	13.36	13.18	13.08	13.02	14.08	14.05	14.03	13.05	13.05
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.750	4.000	4.000	4.250	4.500	4.750	4.750	5.000	5.250	5.500	5.750

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
13.05	13.05	15.87	15.87	15.87	15.88	13.03	13.03	13.03	13.04	13.04
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.000	6.250	6.500	6.750	7.000	7.250	7.500	7.750	8.000	8.250	8.500

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 12
1.000	1.000	1.000	1.000	1.000	1.000	
13.05	13.06	13.09	15.00	15.08	15.22	
1.000	1.000	1.000	1.000	1.000	1.000	
8.750	9.000	9.250	9.500	9.750	10.000	

135 HYDROCYANIC ACID HCN

-1	80.9	9.400	27.03				pHL	3.00	3.25	3.50
							RE	□□□□□□	□□□□□□	□□□□□□
							t	15.14	14.91	14.72
							Z	0.001	0.001	0.002
							pHS	6.443	6.519	6.588

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	96.567	39.822	36.911
14.55	14.40	13.27	13.24	13.22	13.19	14.18	14.17	14.16	13.23	13.23
0.002	0.002	0.004	0.004	0.005	0.005	0.007	0.008	0.010	0.023	0.025
6.663	6.749	6.950	6.997	7.059	7.138	7.237	7.300	7.381	7.772	7.805

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
33.026	28.390	11.914	11.207	10.217	8.972	4.575	4.271	3.864	3.380	2.314
13.22	13.22	15.91	15.91	15.91	15.90	13.17	13.16	13.16	13.16	13.15
0.028	0.033	0.079	0.084	0.092	0.105	0.208	0.223	0.246	0.282	0.415
7.855	7.922	8.319	8.347	8.391	8.453	8.797	8.834	8.890	8.969	9.220

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 4
2.099	1.859	1.624	1.356	1.245	1.152	
13.15	13.16	13.18	15.05	15.12	15.24	
0.458	0.518	0.594	0.715	0.780	0.845	
9.295	9.398	9.530	9.761	9.910	10.093	

136 HYDROFLUORIC ACID (S) HF

-1	57.4	3.173	20.01				pHL	3.00	3.25	3.50
							RE	2.095	1.885	1.734
							t	19.19	17.99	17.19
							Z	0.657	0.732	0.797
							pHS	3.420	3.572	3.729
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.618	1.532	1.519	1.474	1.441	1.420	1.419	1.407	1.399	1.398	1.395
16.61	16.23	14.76	14.57	14.45	14.37	15.84	15.80	15.78	14.42	14.41
0.855	0.904	0.914	0.943	0.965	0.979	0.980	0.988	0.993	0.996	0.998
3.905	4.108	4.159	4.350	4.569	4.804	4.818	5.057	5.303	5.549	5.794
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.394	1.393	1.391	1.391	1.390	1.390	1.393	1.392	1.392	1.392	1.392
14.41	14.41	18.35	18.35	18.35	18.35	14.38	14.38	14.39	14.39	14.40
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.042	6.292	6.561	6.810	7.060	7.310	7.541	7.791	8.041	8.291	8.541
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 7				
1.392	1.392	1.391	1.390	1.390	1.389					
14.41	14.44	14.48	17.17	17.31	17.57					
1.000	1.000	1.000	1.000	1.000	1.000					
8.792	9.042	9.292	9.558	9.809	10.060					

137 HYDROGEN AZIDE HN3

-1	72.0	4.720	43.00				pHL	3.00	3.25	3.50
							RE	5.240	4.433	3.818
							t	16.00	15.60	15.30
							Z	0.204	0.242	0.281
							pHS	4.107	4.200	4.287
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.269	2.763	2.239	2.041	1.831	1.629	1.558	1.430	1.319	1.209	1.175
15.05	14.84	13.57	13.51	13.46	13.41	14.55	14.52	14.50	13.41	13.41
0.329	0.390	0.484	0.532	0.594	0.669	0.701	0.765	0.831	0.909	0.936
4.383	4.497	4.660	4.742	4.850	4.989	5.052	5.193	5.370	5.677	5.843
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.147	1.128	1.115	1.110	1.106	1.104	1.103	1.102	1.102	1.102	1.102
13.40	13.40	16.51	16.51	16.51	16.52	13.38	13.38	13.38	13.39	13.39
0.959	0.976	0.987	0.992	0.996	0.997	0.999	0.999	1.000	1.000	1.000
6.049	6.278	6.548	6.779	7.021	7.268	7.514	7.762	8.011	8.261	8.511
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2				
1.101	1.101	1.101	1.101	1.101	1.101					
13.40	13.42	13.45	15.56	15.65	15.82					
1.000	1.000	1.000	1.000	1.000	1.000					
8.761	9.011	9.261	9.516	9.766	10.016					

138 HYDROGEN HEXAFLUOROPHOSPHIDE HPF6

-1	59.0	0.000	146.00				pHL	3.00	3.25	3.50
							RE	1.353	1.352	1.352
							t	20.61	18.47	17.21
							Z	0.999	1.000	1.000
							pHS	3.094	3.328	3.562
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.352	1.351	1.353	1.353	1.353	1.352	1.352	1.352	1.351	1.353	1.353
16.47	16.05	14.69	14.45	14.31	14.24	15.67	15.63	15.60	14.28	14.27
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.802	4.048	4.049	4.292	4.539	4.787	4.795	5.044	5.294	5.538	5.787
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.353	1.353	1.352	1.352	1.351	1.351	1.353	1.353	1.353	1.353	1.353
14.27	14.27	18.10	18.10	18.10	18.10	14.24	14.25	14.25	14.26	14.26
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.037	6.287	6.555	6.804	7.054	7.304	7.537	7.787	8.037	8.287	8.538
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.353	1.353	1.352	1.352	1.351	1.350					
14.27	14.30	14.34	16.95	17.09	17.33					
1.000	1.000	1.000	1.000	1.000	1.000					
8.788	9.038	9.288	9.552	9.803	10.055					

139 HYDROGEN SULFIDE H2S

-1	67.4	6.960	34.08				pHL	3.00	3.25	3.50
							RE	60.809	50.836	43.172
							t	16.25	15.92	15.66
							Z	0.018	0.022	0.026
							pHS	5.226	5.305	5.377

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
36.218	29.649	19.491	17.435	15.090	12.608	10.373	8.960	7.477	3.801	3.530
15.44	15.25	13.88	13.85	13.81	13.78	14.97	14.95	14.94	13.78	13.77
0.031	0.038	0.058	0.065	0.075	0.089	0.109	0.126	0.152	0.302	0.326
5.455	5.545	5.736	5.787	5.854	5.938	6.033	6.104	6.194	6.572	6.618
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.182	2.787	1.850	1.754	1.635	1.510	1.347	1.300	1.258	1.226	1.206
13.77	13.76	17.03	17.02	17.02	17.02	13.66	13.66	13.66	13.66	13.66
0.362	0.414	0.630	0.665	0.714	0.775	0.873	0.905	0.936	0.960	0.977
6.686	6.780	7.155	7.221	7.320	7.458	7.754	7.895	8.081	8.298	8.549
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 4				
1.195	1.188	1.184	1.181	1.180	1.179					
13.67	13.69	13.72	15.99	16.09	16.28					
0.987	0.992	0.996	0.998	0.999	0.999					
8.782	9.025	9.272	9.529	9.778	10.029					

140 HYDROIODIC ACID HI

-1	79.6	-2.000	127.91				pHL	3.00	3.25	3.50
							RE	0.993	0.993	0.993
							t	18.01	16.22	15.21
							Z	1.000	1.000	1.000
							pHS	2.998	3.248	3.499

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993
14.65	14.33	13.34	13.15	13.05	13.00	14.05	14.02	14.00	13.03	13.03
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.749	3.999	3.999	4.249	4.499	4.749	4.749	4.999	5.249	5.499	5.749
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993
13.02	13.03	15.83	15.83	15.83	15.84	13.00	13.01	13.01	13.02	13.01
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
5.999	6.249	6.499	6.749	6.999	7.249	7.499	7.749	7.999	8.249	8.499
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 12				
0.993	0.993	0.993	0.993	0.993	0.993					
13.02	13.04	13.07	14.96	15.04	15.18					
1.000	1.000	1.000	1.000	1.000	1.000					
8.749	8.999	9.249	9.499	9.749	9.999					

141 2-HYDROXY-3-CHLOROBUTYRIC A. C4H7ClO3

-1	34.4	3.092	138.55				pHL	3.00	3.25	3.50
							RE	3.217	2.958	2.772
							t	26.31	24.12	22.66
							Z	0.728	0.794	0.848
							pHS	3.487	3.643	3.805

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.631	2.528	2.529	2.472	2.432	2.406	2.402	2.387	2.377	2.385	2.381
21.63	20.96	18.49	18.15	17.93	17.79	20.31	20.24	20.19	17.88	17.87
0.896	0.933	0.937	0.959	0.975	0.986	0.986	0.992	0.996	0.997	0.999
3.989	4.198	4.230	4.428	4.651	4.889	4.916	5.158	5.404	5.637	5.883
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.378	2.375	2.367	2.366	2.364	2.362	2.379	2.378	2.376	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.131	6.381	6.683	6.932	7.182	7.432	7.631	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

142 2-HYDROXY-3-Cl-ISOBUTYRIC A. C4H7ClO3

-1 34.4 3.208 138.55

pHL	3.00	3.25	3.50
RE	3.394	3.090	2.870
t	26.11	24.02	22.61
Z	0.689	0.759	0.818
pHS	3.522	3.672	3.827

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.700	2.574	2.569	2.499	2.449	2.416	2.411	2.392	2.380	2.387	2.382
21.62	20.95	18.47	18.15	17.93	17.79	20.31	20.24	20.19	17.88	17.87
0.872	0.916	0.922	0.949	0.968	0.981	0.983	0.990	0.994	0.997	0.998
4.004	4.208	4.245	4.437	4.656	4.891	4.919	5.159	5.405	5.638	5.883
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.379	2.376	2.367	2.366	2.364	2.362	2.379	2.378	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.132	6.381	6.683	6.932	7.182	7.432	7.631	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

143 2-HYDROXY-3-Cl-PROPIONIC A. C3H5ClO3

-1 36.5 3.124 124.52

pHL	3.00	3.25	3.50
RE	3.093	2.830	2.642
t	25.24	23.21	21.85
Z	0.712	0.780	0.837
pHS	3.484	3.638	3.798

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.497	2.392	2.390	2.332	2.291	2.264	2.261	2.245	2.235	2.241	2.237
20.90	20.26	17.94	17.63	17.42	17.29	19.66	19.59	19.55	17.37	17.36
0.887	0.927	0.932	0.956	0.973	0.984	0.985	0.991	0.995	0.997	0.998
3.980	4.188	4.222	4.419	4.641	4.878	4.904	5.145	5.391	5.625	5.871
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.235	2.232	2.225	2.224	2.222	2.221	2.235	2.234	2.233	2.231	2.234
17.35	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.119	6.369	6.667	6.916	7.166	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

144 2-HYDROXY-m-TOLUIC ACID C8H8O3

-1 31.3 3.000 152.15

pHL	3.00	3.25	3.50
RE	3.376	3.138	2.969
t	28.25	25.74	24.08
Z	0.767	0.827	0.875
pHS	3.485	3.645	3.812

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.842	2.751	2.758	2.708	2.673	2.650	2.645	2.631	2.622	2.633	2.630
22.92	22.16	19.45	19.07	18.82	18.67	21.45	21.36	21.32	18.77	18.75
0.916	0.947	0.950	0.968	0.981	0.989	0.989	0.994	0.997	0.998	0.999
4.001	4.214	4.239	4.442	4.668	4.907	4.937	5.179	5.426	5.656	5.903
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.627	2.624	2.613	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

145 3-HYDROXY-o-TOLUIC ACID C8H8O3
-1 31.3 2.983 152.15

pHL	3.00	3.25	3.50
RE	3.354	3.121	2.957
t	28.28	25.76	24.08
Z	0.772	0.831	0.879
pHS	3.480	3.642	3.809

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.834	2.746	2.754	2.705	2.671	2.648	2.643	2.630	2.621	2.633	2.630
22.92	22.16	19.45	19.07	18.82	18.67	21.45	21.36	21.32	18.77	18.75
0.918	0.949	0.951	0.969	0.981	0.989	0.990	0.994	0.997	0.998	0.999
3.999	4.213	4.238	4.441	4.668	4.907	4.936	5.179	5.426	5.656	5.903
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.627	2.623	2.613	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

146 3-HYDROXY-p-TOLUIC ACID C8H8O3
-1 31.3 3.143 152.15

pHL	3.00	3.25	3.50
RE	3.585	3.293	3.082
t	27.99	25.61	24.02
Z	0.721	0.786	0.842
pHS	3.523	3.676	3.835

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.920	2.802	2.804	2.738	2.691	2.660	2.655	2.637	2.625	2.635	2.631
22.90	22.15	19.43	19.06	18.82	18.67	21.45	21.36	21.31	18.77	18.75
0.890	0.929	0.934	0.957	0.974	0.985	0.986	0.992	0.995	0.997	0.998
4.017	4.224	4.255	4.451	4.673	4.910	4.940	5.181	5.427	5.657	5.903
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.627	2.624	2.613	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

147 4-HYDROXY-m-TOLUIC ACID C8H8O3
-1 31.3 3.066 152.15

pHL	3.00	3.25	3.50
RE	3.467	3.205	3.018
t	28.13	25.68	24.05
Z	0.746	0.809	0.861
pHS	3.502	3.659	3.822

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.875	2.773	2.778	2.721	2.681	2.654	2.649	2.633	2.623	2.634	2.630
22.91	22.16	19.44	19.06	18.82	18.67	21.45	21.36	21.32	18.77	18.75
0.905	0.939	0.943	0.963	0.978	0.987	0.988	0.993	0.996	0.998	0.999
4.008	4.218	4.246	4.446	4.670	4.908	4.938	5.180	5.426	5.656	5.903
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.627	2.624	2.613	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

148 6-HYDROXY-o-TOLUIC ACID C8H8O3

-1	31.3	3.321	152.15

pHL	3.00	3.25	3.50
RE	3.908	3.537	3.265
t	27.65	25.43	23.94
Z	0.659	0.730	0.793
pHS	3.577	3.721	3.871

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.051	2.888	2.879	2.790	2.724	2.680	2.672	2.647	2.631	2.639	2.633
22.87	22.14	19.40	19.05	18.81	18.67	21.45	21.36	21.31	18.77	18.75
0.851	0.900	0.908	0.938	0.962	0.977	0.979	0.988	0.993	0.996	0.998
4.042	4.240	4.280	4.466	4.681	4.914	4.945	5.183	5.428	5.659	5.904
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.628	2.625	2.613	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.152	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

149 m-HYDROXYBENZOIC ACID C7H6O3

-1	34.0	4.082	138.12
-2	62.0	9.609	

pHL	3.00	3.25	3.50
RE	6.004	5.154	4.516
t	24.86	23.38	22.36
Z	0.388	0.453	0.518
pHS	3.858	3.973	4.086

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.971	3.503	3.303	3.068	2.856	2.689	2.661	2.559	2.491	2.462	2.439
21.59	21.03	18.40	18.19	18.02	17.90	20.43	20.37	20.33	17.99	17.98
0.592	0.673	0.719	0.776	0.835	0.889	0.898	0.934	0.960	0.977	0.986
4.213	4.364	4.457	4.587	4.752	4.948	4.991	5.198	5.426	5.671	5.899
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.423	2.413	2.398	2.393	2.386	2.377	2.385	2.365	2.332	2.280	2.191
17.97	17.98	24.81	24.83	24.87	24.94	18.19	18.39	18.73	19.29	20.29
0.992	0.996	0.999	1.001	1.004	1.008	1.014	1.025	1.043	1.075	1.135
6.140	6.386	6.691	6.938	7.187	7.436	7.648	7.897	8.146	8.395	8.680
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 2				
2.084	1.955	1.821	1.674	1.583	1.513					
21.47	22.89	24.42	31.18	32.51	33.81					
1.213	1.317	1.443	1.600	1.715	1.812					
8.914	9.145	9.374	9.646	9.866	10.098					

150 p-HYDROXYBENZOIC ACID C7H6O3

-1	34.0	4.530	138.12
-2	62.0	9.310	

pHL	3.00	3.25	3.50
RE	8.759	7.385	6.353
t	24.36	23.07	22.19
Z	0.263	0.313	0.365
pHS	4.062	4.166	4.265

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.455	4.658	4.135	3.765	3.401	3.081	2.999	2.797	2.644	2.544	2.492
21.50	20.99	18.32	18.15	18.01	17.90	20.41	20.36	20.32	17.99	17.98
0.426	0.501	0.570	0.628	0.697	0.772	0.793	0.852	0.903	0.945	0.965
4.375	4.505	4.622	4.725	4.858	5.024	5.078	5.254	5.459	5.721	5.923
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.455	2.430	2.404	2.393	2.381	2.364	2.361	2.324	2.266	2.181	2.046
17.98	17.99	24.84	24.88	24.96	25.11	18.46	18.84	19.44	20.35	21.85
0.979	0.989	0.997	1.002	1.008	1.016	1.028	1.049	1.085	1.140	1.243
6.151	6.391	6.700	6.942	7.189	7.438	7.661	7.909	8.155	8.400	8.689
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 2				
1.921	1.793	1.677	1.567	1.505	1.462					
23.22	24.65	25.98	32.39	33.38	34.37					
1.350	1.475	1.606	1.740	1.828	1.893					
8.908	9.129	9.355	9.620	9.847	10.085					

151 2-HYDROXYBUTYRIC ACID C4H8O3

-1	34.3	3.979	104.11							
							pHL	3.00	3.25	3.50
							RE	5.505	4.751	4.185
							t	24.86	23.33	22.29
							Z	0.420	0.488	0.556
							pHS	3.813	3.931	4.047
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.704	3.296	3.142	2.934	2.752	2.611	2.589	2.505	2.450	2.429	2.410
21.50	20.93	18.34	18.12	17.94	17.82	20.33	20.27	20.22	17.91	17.90
0.630	0.710	0.750	0.805	0.860	0.908	0.915	0.946	0.968	0.981	0.989
4.179	4.336	4.423	4.560	4.732	4.935	4.975	5.188	5.420	5.663	5.894
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.398	2.390	2.378	2.375	2.372	2.370	2.387	2.385	2.384	2.382	2.385
17.89	17.88	24.63	24.63	24.63	24.62	17.85	17.85	17.86	17.87	17.89
0.994	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.136	6.383	6.686	6.934	7.183	7.433	7.632	7.881	8.131	8.381	8.633
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 3				
2.383	2.381	2.379	2.372	2.369	2.366					
17.92	17.98	18.08	22.85	23.29	24.13					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.134	9.385	9.683	9.937	10.196					

152 3-HYDROXYBUTYRIC ACID C4H8O3

-1	34.3	4.519	104.11							
							pHL	3.00	3.25	3.50
							RE	8.608	7.260	6.247
							t	24.23	22.95	22.07
							Z	0.266	0.316	0.368
							pHS	4.056	4.160	4.260
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.367	4.585	4.074	3.711	3.354	3.041	2.962	2.765	2.615	2.518	2.468
21.39	20.88	18.24	18.07	17.93	17.82	20.31	20.26	20.22	17.91	17.90
0.430	0.505	0.573	0.631	0.700	0.775	0.795	0.854	0.904	0.945	0.965
4.370	4.500	4.617	4.720	4.854	5.020	5.074	5.250	5.456	5.718	5.920
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.433	2.410	2.388	2.381	2.376	2.372	2.388	2.386	2.384	2.382	2.385
17.89	17.88	24.63	24.63	24.62	24.62	17.85	17.85	17.86	17.87	17.89
0.979	0.988	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.148	6.389	6.694	6.937	7.184	7.433	7.632	7.882	8.131	8.381	8.633
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 3				
2.383	2.381	2.379	2.372	2.369	2.366					
17.92	17.98	18.08	22.85	23.29	24.13					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.134	9.385	9.683	9.937	10.196					

153 4-HYDROXYBUTYRIC ACID C4H8O3

-1	34.3	4.721	104.11							
							pHL	3.00	3.25	3.50
							RE	10.360	8.687	7.430
							t	24.06	22.85	22.01
							Z	0.220	0.263	0.308
							pHS	4.151	4.252	4.347
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.334	5.350	4.614	4.173	3.729	3.325	3.202	2.943	2.737	2.581	2.512
21.36	20.87	18.21	18.06	17.93	17.82	20.30	20.25	20.22	17.91	17.90
0.362	0.431	0.504	0.559	0.627	0.706	0.734	0.800	0.862	0.921	0.947
4.452	4.574	4.700	4.794	4.916	5.068	5.128	5.289	5.481	5.752	5.939
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.460	2.426	2.396	2.385	2.378	2.373	2.389	2.387	2.385	2.382	2.385
17.89	17.89	24.63	24.63	24.62	24.62	17.85	17.85	17.86	17.87	17.89
0.968	0.981	0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.157	6.393	6.700	6.939	7.185	7.434	7.633	7.882	8.131	8.381	8.633
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 3				
2.384	2.381	2.379	2.372	2.369	2.366					
17.92	17.98	18.08	22.85	23.29	24.13					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.134	9.385	9.683	9.937	10.196					

154 m-HYDROXYCINNAMIC ACID C9H803
-1 27.0 4.397 164.16

pHL	3.00	3.25	3.50
RE	9.479	8.045	6.961
t	28.86	27.02	25.77
Z	0.309	0.366	0.424
pHS	4.027	4.135	4.240

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.025	5.203	4.795	4.386	4.001	3.680	3.606	3.407	3.265	3.195	3.146
24.83	24.14	20.80	20.56	20.36	20.22	23.43	23.36	23.31	20.35	20.34
0.492	0.572	0.627	0.688	0.757	0.825	0.841	0.892	0.932	0.960	0.975
4.358	4.496	4.593	4.709	4.857	5.037	5.088	5.281	5.498	5.744	5.960
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.112	3.091	3.062	3.055	3.050	3.045	3.076	3.074	3.071	3.067	3.072
20.32	20.32	28.99	28.99	28.98	28.97	20.28	20.28	20.29	20.31	20.34
0.986	0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.196	6.439	6.758	7.004	7.252	7.501	7.686	7.935	8.185	8.435	8.688
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.069	3.066	3.061	3.048	3.042	3.034					
20.39	20.49	20.66	26.97	27.80	29.48					
1.000	1.000	1.000	1.000	1.000	1.000					
8.938	9.189	9.442	9.758	10.016	10.282					

155 o-HYDROXYCINNAMIC ACID C9H803
-1 27.0 4.613 164.16

pHL	3.00	3.25	3.50
RE	11.491	9.674	8.302
t	28.60	26.85	25.66
Z	0.254	0.302	0.354
pHS	4.125	4.229	4.329

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.110	6.052	5.420	4.911	4.416	3.983	3.867	3.592	3.386	3.261	3.189
24.76	24.10	20.74	20.52	20.34	20.21	23.41	23.35	23.30	20.35	20.33
0.415	0.489	0.552	0.611	0.683	0.759	0.782	0.844	0.897	0.940	0.961
4.440	4.569	4.676	4.780	4.914	5.079	5.136	5.313	5.518	5.772	5.974
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.139	3.106	3.070	3.060	3.052	3.046	3.077	3.074	3.071	3.067	3.072
20.32	20.32	28.99	28.99	28.98	28.97	20.28	20.28	20.29	20.31	20.34
0.977	0.987	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.202	6.442	6.762	7.005	7.252	7.501	7.686	7.935	8.185	8.435	8.688
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.069	3.066	3.061	3.048	3.042	3.034					
20.39	20.49	20.66	26.97	27.80	29.48					
1.000	1.000	1.000	1.000	1.000	1.000					
8.938	9.189	9.442	9.758	10.016	10.282					

156 p-HYDROXYCINNAMIC ACID C9H803
-1 27.0 4.678 164.16

pHL	3.00	3.25	3.50
RE	12.202	10.251	8.777
t	28.53	26.80	25.63
Z	0.239	0.285	0.334
pHS	4.156	4.259	4.357

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.496	6.356	5.642	5.100	4.567	4.096	3.963	3.663	3.434	3.286	3.206
24.74	24.09	20.72	20.52	20.34	20.21	23.41	23.34	23.30	20.35	20.33
0.393	0.465	0.530	0.588	0.659	0.737	0.762	0.827	0.884	0.932	0.956
4.465	4.592	4.702	4.803	4.934	5.094	5.153	5.324	5.526	5.782	5.979
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.149	3.112	3.073	3.061	3.053	3.047	3.077	3.074	3.071	3.067	3.072
20.32	20.32	28.99	28.99	28.98	28.97	20.28	20.28	20.29	20.31	20.34
0.973	0.984	0.992	0.996	0.998	0.999	0.999	0.999	1.000	1.000	1.000
6.205	6.444	6.763	7.006	7.253	7.501	7.686	7.935	8.185	8.435	8.688
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 7				
3.069	3.066	3.061	3.048	3.042	3.034					
20.39	20.49	20.66	26.97	27.80	29.48					
1.000	1.000	1.000	1.000	1.000	1.000					
8.938	9.189	9.442	9.758	10.016	10.282					

157 2-HYDROXYISOBUTYRIC ACID (S) C4H8O3

-1	33.5	3.971	104.11				pHL	3.00	3.25	3.50
							RE	5.585	4.824	4.252
							t	25.27	23.69	22.62
							Z	0.424	0.493	0.561
							pHS	3.812	3.931	4.048

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.767	3.356	3.206	2.996	2.812	2.671	2.648	2.564	2.509	2.489	2.470
21.81	21.22	18.57	18.34	18.16	18.03	20.61	20.54	20.49	18.12	18.11
0.635	0.715	0.754	0.809	0.863	0.910	0.917	0.948	0.969	0.982	0.989
4.180	4.338	4.423	4.561	4.735	4.939	4.978	5.193	5.425	5.666	5.898

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.458	2.450	2.437	2.434	2.432	2.429	2.447	2.446	2.444	2.442	2.445
18.10	18.10	25.02	25.01	25.01	25.00	18.06	18.06	18.07	18.08	18.10
0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.141	6.388	6.693	6.940	7.190	7.439	7.637	7.886	8.136	8.386	8.638

8.75	9.00	9.25	9.50	9.75	10.00
2.443	2.441	2.438	2.432	2.428	2.424
18.13	18.20	18.30	23.20	23.67	24.56
1.000	1.000	1.000	1.000	1.000	1.000
8.888	9.139	9.390	9.690	9.944	10.203

(Ref.) : 11 , 4

158 p-HYDROXYPHENYLACETIC ACID C8H8O3

-1	26.9	3.171	152.15				pHL	3.00	3.25	3.50
							RE	4.162	3.835	3.597
							t	31.17	28.40	26.55
							Z	0.727	0.791	0.845
							pHS	3.566	3.718	3.876

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.414	3.279	3.287	3.212	3.158	3.122	3.113	3.092	3.078	3.094	3.089
25.23	24.36	21.17	20.74	20.45	20.27	23.54	23.44	23.38	20.40	20.38
0.892	0.930	0.935	0.957	0.974	0.985	0.986	0.992	0.995	0.997	0.998
4.056	4.263	4.292	4.487	4.708	4.944	4.979	5.219	5.465	5.692	5.938

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.084	3.080	3.063	3.061	3.058	3.055	3.087	3.085	3.082	3.079	3.084
20.37	20.36	29.07	29.06	29.06	29.05	20.32	20.33	20.34	20.35	20.38
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.186	6.435	6.753	7.002	7.252	7.502	7.686	7.936	8.186	8.436	8.688

8.75	9.00	9.25	9.50	9.75	10.00
3.081	3.078	3.073	3.060	3.054	3.045
20.44	20.53	20.71	27.05	27.88	29.58
1.000	1.000	1.000	1.000	1.000	1.000
8.939	9.190	9.443	9.759	10.018	10.284

(Ref.) : 11 , 2

159 HYDROXYTRIMETHYLACETIC ACID C5H10O3

-1	31.3	4.863	118.13				pHL	3.00	3.25	3.50
							RE	12.834	10.722	9.134
							t	25.50	24.16	23.23
							Z	0.194	0.233	0.274
							pHS	4.227	4.327	4.420

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.749	6.503	5.543	4.986	4.422	3.902	3.727	3.393	3.119	2.898	2.806
22.52	21.98	19.06	18.91	18.77	18.66	21.38	21.33	21.30	18.76	18.75
0.324	0.388	0.460	0.513	0.580	0.660	0.692	0.762	0.831	0.903	0.933
4.522	4.641	4.767	4.857	4.974	5.120	5.183	5.336	5.521	5.794	5.971

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.735	2.687	2.643	2.629	2.619	2.612	2.632	2.630	2.627	2.624	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.958	0.975	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.184	6.416	6.729	6.966	7.211	7.459	7.653	7.902	8.151	8.401	8.653

8.75	9.00	9.25	9.50	9.75	10.00
2.625	2.622	2.619	2.611	2.607	2.601
18.79	18.86	18.98	24.28	24.83	25.91
1.000	1.000	1.000	1.000	1.000	1.000
8.903	9.154	9.406	9.710	9.966	10.226

(Ref.) : 3

160 2-HYDROXYVALERIC ACID C5H1003

-1	32.3	3.886	118.13				pHL	3.00	3.25	3.50
							RE	5.414	4.702	4.168
							t	26.05	24.34	23.18
							Z	0.455	0.526	0.595
							pHS	3.782	3.903	4.024

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.717	3.340	3.222	3.026	2.858	2.733	2.714	2.640	2.592	2.579	2.562
22.31	21.69	18.95	18.69	18.50	18.36	21.04	20.97	20.93	18.46	18.45
0.669	0.748	0.781	0.833	0.883	0.925	0.930	0.957	0.974	0.985	0.991
4.161	4.325	4.403	4.548	4.728	4.937	4.976	5.195	5.430	5.669	5.904
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.551	2.544	2.531	2.528	2.526	2.523	2.543	2.542	2.540	2.537	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.148	6.395	6.702	6.950	7.199	7.449	7.644	7.894	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

161 4-HYDROXYVALERIC ACID C5H1003

-1	32.3	4.699	118.13				pHL	3.00	3.25	3.50
							RE	10.690	8.968	7.674
							t	25.08	23.75	22.83
							Z	0.227	0.271	0.317
							pHS	4.146	4.248	4.344

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.547	5.538	4.819	4.359	3.899	3.484	3.362	3.097	2.888	2.737	2.667
22.13	21.60	18.78	18.62	18.47	18.36	21.01	20.95	20.92	18.46	18.45
0.373	0.443	0.514	0.570	0.639	0.718	0.744	0.810	0.870	0.926	0.951
4.450	4.574	4.695	4.791	4.916	5.071	5.130	5.294	5.490	5.757	5.947
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.615	2.581	2.549	2.539	2.532	2.526	2.545	2.543	2.540	2.538	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.970	0.982	0.991	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.168	6.405	6.715	6.955	7.202	7.450	7.646	7.895	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

162 HYPOPHOSPHOROUS ACID (S) H3PO2

-1	45.2	1.230	66.00				pHL	3.00	3.25	3.50
							RE	1.798	1.791	1.787
							t	23.64	21.13	19.61
							Z	0.990	0.994	0.996
							pHS	3.192	3.409	3.629

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.784	1.782	1.787	1.786	1.785	1.784	1.783	1.782	1.781	1.786	1.786
18.68	18.12	16.32	16.01	15.83	15.73	17.62	17.57	17.54	15.79	15.78
0.998	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.860	4.100	4.104	4.339	4.582	4.829	4.845	5.093	5.343	5.580	5.829
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.785	1.784	1.781	1.780	1.780	1.779	1.786	1.786	1.785	1.784	1.785
15.78	15.78	20.83	20.83	20.83	20.83	15.75	15.75	15.76	15.76	15.77
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.079	6.329	6.613	6.863	7.113	7.363	7.579	7.829	8.079	8.329	8.580
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 4				
1.785	1.784	1.783	1.780	1.779	1.777					
15.79	15.83	15.89	19.38	19.62	20.04					
1.000	1.000	1.000	1.000	1.000	1.000					
8.830	9.080	9.331	9.610	9.862	10.116					

163 IODIC ACID HIO2

-1 42.0 0.770 159.91

pHL	3.00	3.25	3.50
RE	1.928	1.926	1.924
t	24.69	22.03	20.41
Z	0.997	0.998	0.999
pHS	3.213	3.429	3.647

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.923	1.922	1.928	1.928	1.927	1.925	1.924	1.923	1.922	1.929	1.928
19.41	18.81	16.86	16.53	16.34	16.22	18.27	18.21	18.17	16.29	16.28
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.876	4.116	4.119	4.352	4.595	4.842	4.861	5.108	5.358	5.593	5.842

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.927	1.926	1.922	1.921	1.920	1.919	1.929	1.928	1.927	1.926	1.928
16.28	16.28	21.74	21.74	21.73	21.73	16.24	16.25	16.25	16.26	16.27
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.092	6.342	6.631	6.881	7.130	7.380	7.592	7.842	8.092	8.342	8.593

8.75	9.00	9.25	9.50	9.75	10.00
1.927	1.926	1.924	1.921	1.920	1.917
16.29	16.33	16.41	20.20	20.47	20.98
1.000	1.000	1.000	1.000	1.000	1.000
8.843	9.094	9.344	9.628	9.881	10.136

(Ref.) : 1 , 4

164 IODOACETIC ACID C2H3IO2

-1 42.1 3.174 185.95

pHL	3.00	3.25	3.50
RE	2.782	2.524	2.338
t	22.95	21.25	20.11
Z	0.682	0.753	0.814
pHS	3.471	3.623	3.780

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.195	2.089	2.081	2.024	1.982	1.956	1.953	1.938	1.928	1.930	1.927
19.31	18.77	16.76	16.49	16.32	16.21	18.25	18.19	18.15	16.28	16.27
0.869	0.914	0.921	0.948	0.968	0.981	0.982	0.990	0.994	0.997	0.998
3.959	4.163	4.204	4.397	4.617	4.853	4.875	5.115	5.360	5.599	5.844

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.924	1.922	1.918	1.917	1.916	1.915	1.924	1.923	1.923	1.921	1.923
16.26	16.26	21.71	21.70	21.70	21.70	16.23	16.23	16.24	16.25	16.25
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.092	6.342	6.631	6.880	7.130	7.380	7.591	7.841	8.091	8.342	8.593

8.75	9.00	9.25	9.50	9.75	10.00
1.922	1.921	1.920	1.916	1.915	1.913
16.28	16.32	16.39	20.17	20.44	20.95
1.000	1.000	1.000	1.000	1.000	1.000
8.843	9.093	9.344	9.628	9.880	10.135

(Ref.) : 1

165 m-IODOBENZOIC ACID C7H5IO2

-1 33.4 3.851 248.02

pHL	3.00	3.25	3.50
RE	5.129	4.461	3.960
t	25.50	23.85	22.72
Z	0.465	0.536	0.605
pHS	3.762	3.885	4.007

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.539	3.188	3.080	2.898	2.742	2.627	2.610	2.542	2.499	2.487	2.472
21.87	21.27	18.63	18.38	18.19	18.06	20.64	20.57	20.53	18.15	18.14
0.679	0.757	0.789	0.840	0.889	0.929	0.934	0.959	0.976	0.986	0.992
4.146	4.311	4.388	4.535	4.717	4.928	4.965	5.186	5.422	5.661	5.896

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.462	2.455	2.444	2.441	2.439	2.436	2.455	2.453	2.452	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.141	6.388	6.693	6.941	7.190	7.440	7.637	7.887	8.137	8.387	8.639

8.75	9.00	9.25	9.50	9.75	10.00
2.451	2.449	2.446	2.439	2.436	2.432
18.16	18.22	18.33	23.25	23.72	24.62
1.000	1.000	1.000	1.000	1.000	1.000
8.889	9.140	9.391	9.691	9.945	10.204

(Ref.) : 3 , 1

166 o-IODOBENZOIC ACID C7H5IO2

-1	33.4	2.863	248.02				pHL	3.00	3.25	3.50
							RE	3.023	2.835	2.703
							t	27.24	24.78	23.16
							Z	0.802	0.856	0.899
							pHS	3.436	3.603	3.778

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.607	2.540	2.548	2.510	2.485	2.468	2.464	2.454	2.447	2.458	2.455
22.04	21.32	18.80	18.43	18.20	18.06	20.66	20.58	20.53	18.15	18.14
0.933	0.959	0.961	0.975	0.985	0.992	0.992	0.995	0.997	0.998	0.999
3.973	4.191	4.213	4.421	4.651	4.892	4.919	5.163	5.410	5.641	5.888
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.452	2.450	2.441	2.440	2.438	2.436	2.454	2.453	2.451	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.137	6.387	6.691	6.940	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

167 p-IODOBENZOIC ACID C7H5IO2

-1	33.4	3.930	248.02				pHL	3.00	3.25	3.50
							RE	5.432	4.702	4.155
							t	25.38	23.78	22.68
							Z	0.438	0.507	0.576
							pHS	3.795	3.915	4.034

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.692	3.301	3.166	2.966	2.792	2.660	2.640	2.561	2.510	2.493	2.476
21.85	21.26	18.61	18.37	18.18	18.06	20.64	20.57	20.53	18.15	18.14
0.650	0.730	0.766	0.820	0.872	0.917	0.923	0.952	0.971	0.983	0.990
4.169	4.329	4.411	4.552	4.729	4.935	4.974	5.191	5.424	5.665	5.898
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.464	2.457	2.444	2.441	2.439	2.436	2.455	2.453	2.452	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.141	6.389	6.693	6.941	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

168 4-IODOBUTYRIC ACID C4H7IO2

-1	34.4	4.638	214.00				pHL	3.00	3.25	3.50
							RE	9.566	8.039	6.892
							t	24.08	22.85	22.00
							Z	0.238	0.283	0.332
							pHS	4.111	4.214	4.310

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.893	5.000	4.364	3.958	3.553	3.189	3.086	2.855	2.674	2.545	2.484
21.34	20.84	18.19	18.04	17.90	17.80	20.28	20.22	20.19	17.88	17.87
0.389	0.460	0.532	0.588	0.658	0.735	0.760	0.823	0.881	0.932	0.955
4.417	4.542	4.665	4.763	4.889	5.047	5.104	5.271	5.469	5.737	5.930
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.440	2.411	2.385	2.376	2.370	2.365	2.381	2.379	2.377	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.973	0.984	0.992	0.995	0.997	0.999	0.999	0.999	1.000	1.000	1.000
6.153	6.391	6.696	6.938	7.184	7.433	7.632	7.881	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

169 m-IODOPHENYLACETIC ACID C8H7IO2

-1	34.3	4.159	262.05				pHL	3.00	3.25	3.50
							RE	6.334	5.418	4.729
							t	24.62	23.19	22.21
							Z	0.364	0.426	0.490
							pHS	3.891	4.004	4.114
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.138	3.627	3.386	3.133	2.901	2.713	2.679	2.565	2.486	2.450	2.423
21.46	20.92	18.30	18.10	17.94	17.82	20.33	20.26	20.22	17.91	17.90
0.562	0.643	0.694	0.752	0.814	0.872	0.883	0.923	0.953	0.973	0.984
4.238	4.384	4.482	4.607	4.766	4.957	5.001	5.203	5.428	5.676	5.900
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.405	2.394	2.380	2.376	2.373	2.370	2.387	2.386	2.384	2.382	2.385
17.89	17.88	24.63	24.63	24.63	24.62	17.85	17.85	17.86	17.87	17.89
0.991	0.995	0.997	0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.139	6.384	6.688	6.935	7.183	7.433	7.632	7.881	8.131	8.381	8.633
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.383	2.381	2.379	2.372	2.369	2.366					
17.92	17.98	18.08	22.85	23.29	24.13					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.134	9.385	9.683	9.937	10.196					

170 o-IODOPHENYLACETIC ACID C8H7IO2

-1	34.3	4.038	262.05				pHL	3.00	3.25	3.50
							RE	5.758	4.954	4.350
							t	24.77	23.28	22.26
							Z	0.401	0.467	0.534
							pHS	3.838	3.954	4.069
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.835	3.395	3.216	2.994	2.796	2.641	2.616	2.522	2.460	2.435	2.414
21.49	20.93	18.33	18.12	17.94	17.82	20.33	20.27	20.22	17.91	17.90
0.608	0.689	0.733	0.789	0.846	0.897	0.905	0.940	0.964	0.979	0.987
4.198	4.351	4.442	4.575	4.742	4.942	4.983	5.193	5.422	5.666	5.896
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.400	2.391	2.378	2.375	2.373	2.370	2.387	2.386	2.384	2.382	2.385
17.89	17.88	24.63	24.63	24.63	24.62	17.85	17.85	17.86	17.87	17.89
0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.137	6.384	6.687	6.934	7.183	7.433	7.632	7.881	8.131	8.381	8.633
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.383	2.381	2.379	2.372	2.369	2.366					
17.92	17.98	18.08	22.85	23.29	24.13					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.134	9.385	9.683	9.937	10.196					

171 p-IODOPHENYLACETIC ACID C8H7IO2

-1	34.3	4.178	262.05				pHL	3.00	3.25	3.50
							RE	6.432	5.497	4.793
							t	24.59	23.17	22.20
							Z	0.358	0.420	0.483
							pHS	3.900	4.012	4.121
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.190	3.666	3.415	3.157	2.919	2.726	2.690	2.572	2.491	2.452	2.425
21.46	20.92	18.30	18.10	17.94	17.82	20.33	20.26	20.22	17.91	17.90
0.555	0.636	0.688	0.746	0.809	0.868	0.879	0.921	0.951	0.972	0.983
4.244	4.390	4.489	4.612	4.770	4.959	5.004	5.205	5.429	5.677	5.900
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.406	2.395	2.380	2.376	2.373	2.370	2.387	2.386	2.384	2.382	2.385
17.89	17.88	24.63	24.63	24.63	24.62	17.85	17.85	17.86	17.87	17.89
0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.139	6.385	6.688	6.935	7.183	7.433	7.632	7.881	8.131	8.381	8.633
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.383	2.381	2.379	2.372	2.369	2.366					
17.92	17.98	18.08	22.85	23.29	24.13					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.134	9.385	9.683	9.937	10.196					

172 3-IODOPROPIONIC ACID C3H5IO2

-1	36.5	4.056	199.98				pHL	3.00	3.25	3.50
							RE	5.531	4.750	4.164
							t	23.74	22.38	21.44
							Z	0.391	0.457	0.523
							pHS	3.839	3.954	4.067
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.665	3.236	3.048	2.834	2.642	2.490	2.465	2.373	2.311	2.284	2.263
20.73	20.21	17.76	17.57	17.41	17.29	19.65	19.58	19.55	17.37	17.36
0.596	0.677	0.724	0.780	0.839	0.891	0.900	0.936	0.961	0.978	0.987
4.194	4.345	4.441	4.571	4.736	4.933	4.974	5.181	5.410	5.656	5.884
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.249	2.241	2.229	2.226	2.224	2.221	2.236	2.235	2.233	2.231	2.234
17.36	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.125	6.371	6.671	6.918	7.167	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

173 5-IODOVALERIC ACID C5H9IO2

-1	32.3	4.770	228.03				pHL	3.00	3.25	3.50
							RE	11.429	9.570	8.173
							t	25.02	23.71	22.81
							Z	0.212	0.253	0.297
							pHS	4.180	4.280	4.375
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.955	5.862	5.048	4.556	4.059	3.607	3.465	3.175	2.943	2.765	2.686
22.12	21.59	18.77	18.61	18.47	18.36	21.00	20.95	20.92	18.46	18.45
0.351	0.418	0.490	0.544	0.613	0.692	0.721	0.789	0.853	0.916	0.943
4.479	4.601	4.725	4.818	4.939	5.090	5.150	5.309	5.500	5.771	5.955
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.627	2.588	2.553	2.541	2.533	2.527	2.546	2.543	2.541	2.538	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.965	0.979	0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.172	6.407	6.717	6.956	7.202	7.450	7.646	7.895	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

174 ISOBUTYRIC ACID C4H8O2

-1	34.4	4.860	88.11				pHL	3.00	3.25	3.50
							RE	11.795	9.857	8.402
							t	23.92	22.74	21.93
							Z	0.192	0.230	0.271
							pHS	4.217	4.316	4.409
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.130	5.984	5.054	4.552	4.040	3.564	3.401	3.095	2.842	2.629	2.545
21.30	20.82	18.16	18.02	17.90	17.80	20.27	20.22	20.19	17.88	17.87
0.320	0.383	0.458	0.509	0.576	0.655	0.687	0.757	0.826	0.901	0.931
4.510	4.628	4.759	4.847	4.962	5.106	5.169	5.320	5.502	5.781	5.955
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.479	2.435	2.396	2.383	2.374	2.367	2.382	2.380	2.378	2.375	2.378
17.86	17.86	24.59	24.58	24.58	24.57	17.82	17.83	17.83	17.84	17.86
0.957	0.974	0.987	0.992	0.996	0.998	0.998	0.999	1.000	1.000	1.000
6.166	6.397	6.705	6.941	7.186	7.433	7.633	7.882	8.131	8.381	8.632
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 7				
2.376	2.374	2.372	2.365	2.362	2.358					
17.89	17.95	18.06	22.80	23.24	24.08					
1.000	1.000	1.000	1.000	1.000	1.000					
8.883	9.133	9.385	9.682	9.936	10.195					

175 ISOCAPROIC ACID C6H12O2

-1	30.3	4.845	116.16				pHL	3.00	3.25	3.50
							RE	12.968	10.838	9.236
							t	26.10	24.69	23.72
							Z	0.199	0.238	0.281
							pHS	4.222	4.322	4.416

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.839	6.585	5.646	5.080	4.508	3.984	3.812	3.475	3.202	2.987	2.895
22.97	22.41	19.40	19.24	19.09	18.98	21.80	21.75	21.71	19.09	19.08
0.332	0.397	0.467	0.521	0.589	0.669	0.700	0.770	0.838	0.906	0.936
4.519	4.639	4.761	4.853	4.972	5.119	5.182	5.337	5.524	5.795	5.975
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.824	2.777	2.733	2.719	2.709	2.702	2.724	2.721	2.718	2.715	2.719
19.07	19.06	26.75	26.74	26.74	26.73	19.03	19.03	19.04	19.05	19.07
0.960	0.976	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.189	6.422	6.737	6.975	7.220	7.468	7.660	7.909	8.158	8.408	8.660
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.717	2.714	2.710	2.701	2.697	2.691					
19.12	19.19	19.32	24.83	25.43	26.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.911	9.162	9.413	9.720	9.976	10.238					

176 ISOCITRIC ACID C6H8O7

-1	29.0	3.250	192.13				pHL	3.00	3.25	3.50
-2	55.0	4.720					RE	3.728	3.316	2.989
-3	74.0	6.380					t	30.79	28.83	27.84
							Z	0.761	0.862	0.965
							pHS	3.559	3.707	3.858

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.698	2.432	2.364	2.178	2.004	1.854	1.831	1.722	1.632	1.563	1.505
27.59	28.03	25.33	26.16	27.21	28.38	31.88	33.07	34.38	33.02	34.56
1.082	1.218	1.269	1.399	1.545	1.699	1.720	1.860	1.999	2.167	2.308
4.030	4.222	4.291	4.465	4.661	4.875	4.908	5.122	5.351	5.627	5.846
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.449	1.400	1.344	1.319	1.300	1.287	1.309	1.305	1.301	1.298	1.300
36.24	37.83	49.70	50.64	51.28	51.66	41.30	41.43	41.51	41.56	41.61
2.461	2.610	2.756	2.841	2.903	2.943	2.967	2.981	2.989	2.994	2.997
6.076	6.313	6.597	6.824	7.063	7.308	7.547	7.794	8.042	8.292	8.542
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 4				
1.298	1.296	1.294	1.280	1.277	1.274					
41.65	41.71	41.81	49.10	49.42	50.02					
2.998	2.999	2.999	3.000	3.000	3.000					
8.792	9.042	9.292	9.553	9.803	10.054					

177 ISOPHTHALIC ACID C8H6O4

-1	28.0	3.720	166.13				pHL	3.00	3.25	3.50
-2	53.0	4.600					RE	4.711	4.007	3.469
							t	31.55	30.03	29.28
							Z	0.625	0.741	0.866
							pHS	3.712	3.835	3.959

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.007	2.611	2.481	2.261	2.070	1.923	1.902	1.810	1.749	1.727	1.706
29.09	29.42	26.59	27.16	27.86	28.56	32.09	32.63	33.03	30.16	30.30
1.012	1.183	1.265	1.405	1.555	1.694	1.711	1.811	1.884	1.933	1.960
4.099	4.263	4.342	4.490	4.670	4.877	4.908	5.123	5.354	5.604	5.836
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.692	1.683	1.667	1.663	1.660	1.656	1.680	1.678	1.677	1.675	1.678
30.39	30.44	39.85	39.85	39.84	39.82	30.47	30.48	30.48	30.49	30.51
1.977	1.987	1.993	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000
6.079	6.326	6.607	6.854	7.103	7.352	7.574	7.823	8.073	8.323	8.574
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
1.676	1.674	1.672	1.661	1.658	1.654					
30.54	30.60	30.70	37.15	37.52	38.23					
2.000	2.000	2.000	2.000	2.000	2.000					
8.824	9.074	9.325	9.600	9.851	10.104					

178 o-ISOPROPYLBENZOIC ACID C10H12O2

-1	24.7	3.635	164.20				pHL	3.00	3.25	3.50
							RE	5.753	5.118	4.642
							t	32.26	29.66	27.90
							Z	0.570	0.643	0.711
							pHS	3.730	3.862	3.997

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.251	3.939	3.903	3.731	3.596	3.502	3.483	3.429	3.395	3.404	3.392
26.61	25.73	22.18	21.78	21.49	21.30	24.87	24.77	24.70	21.45	21.43
0.779	0.844	0.858	0.899	0.934	0.960	0.963	0.978	0.987	0.992	0.996
4.152	4.335	4.384	4.553	4.754	4.979	5.018	5.251	5.493	5.720	5.961
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.383	3.375	3.352	3.349	3.346	3.342	3.381	3.379	3.375	3.371	3.378
21.41	21.40	30.93	30.92	30.91	30.90	21.37	21.37	21.38	21.40	21.44
0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.208	6.457	6.779	7.029	7.278	7.528	7.707	7.957	8.207	8.457	8.710
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.374	3.370	3.364	3.346	3.339	3.328					
21.50	21.62	21.83	28.87	29.94	32.19					
1.000	1.000	1.000	1.000	1.000	1.000					
8.961	9.212	9.465	9.790	10.050	10.320					

179 p-ISOPROPYLBENZOIC ACID C10H12O2

-1	24.7	4.354	164.20				pHL	3.00	3.25	3.50
							RE	9.836	8.376	7.267
							t	30.93	28.84	27.42
							Z	0.327	0.386	0.446
							pHS	4.020	4.130	4.236

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.310	5.476	5.108	4.683	4.289	3.966	3.893	3.694	3.556	3.496	3.448
26.36	25.59	21.94	21.67	21.44	21.29	24.82	24.74	24.69	21.44	21.42
0.516	0.598	0.647	0.708	0.776	0.842	0.857	0.904	0.940	0.965	0.979
4.357	4.499	4.588	4.709	4.862	5.047	5.098	5.296	5.518	5.757	5.978
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.415	3.394	3.361	3.354	3.349	3.343	3.382	3.379	3.376	3.372	3.378
21.41	21.40	30.93	30.92	30.91	30.90	21.37	21.37	21.38	21.40	21.44
0.987	0.993	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.216	6.460	6.784	7.030	7.279	7.528	7.707	7.957	8.207	8.457	8.710
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
3.374	3.370	3.364	3.346	3.339	3.328					
21.50	21.62	21.83	28.87	29.94	32.19					
1.000	1.000	1.000	1.000	1.000	1.000					
8.961	9.212	9.465	9.790	10.050	10.320					

180 ISOPROPYLMALONIC ACID C6H10O4

-1	26.0	2.943	146.14				pHL	3.00	3.25	3.50
-2	52.0	5.879					RE	3.901	3.658	3.480
							t	32.50	29.47	27.49
							Z	0.807	0.863	0.909
							pHS	3.519	3.682	3.851

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.337	3.218	3.226	3.127	3.012	2.866	2.831	2.654	2.455	2.211	2.079
26.19	25.48	22.21	22.08	22.33	22.97	26.57	27.60	28.84	27.43	28.29
0.950	0.987	0.992	1.025	1.067	1.125	1.138	1.221	1.328	1.505	1.610
4.043	4.257	4.287	4.492	4.718	4.952	4.998	5.225	5.450	5.757	5.938
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.962	1.869	1.781	1.747	1.723	1.707	1.725	1.719	1.715	1.712	1.714
29.06	29.67	39.70	39.93	40.07	40.14	30.65	30.68	30.70	30.72	30.75
1.716	1.809	1.894	1.933	1.960	1.977	1.986	1.992	1.996	1.997	1.999
6.142	6.363	6.663	6.882	7.118	7.362	7.584	7.829	8.078	8.327	8.578
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 2				
1.712	1.709	1.707	1.696	1.692	1.689					
30.79	30.84	30.95	37.54	37.93	38.67					
1.999	2.000	2.000	2.000	2.000	2.000					
8.828	9.078	9.328	9.604	9.856	10.109					

181 ISOVALERIC ACID C5H1002

-1	32.1	4.780			102.13		pHL	3.00	3.25	3.50
							RE	11.600	9.710	8.291
							t	25.12	23.80	22.90
							Z	0.210	0.251	0.295
							pHS	4.185	4.286	4.380

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.053	5.942	5.112	4.612	4.107	3.647	3.501	3.206	2.969	2.787	2.707
22.20	21.67	18.83	18.67	18.53	18.42	21.08	21.03	20.99	18.52	18.51
0.348	0.415	0.487	0.541	0.610	0.689	0.718	0.787	0.851	0.915	0.942
4.484	4.605	4.729	4.823	4.943	5.093	5.154	5.313	5.503	5.773	5.957
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.646	2.606	2.570	2.558	2.549	2.544	2.562	2.560	2.557	2.555	2.558
18.50	18.49	25.73	25.72	25.72	25.71	18.46	18.46	18.47	18.48	18.50
0.964	0.979	0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.174	6.408	6.719	6.958	7.204	7.452	7.647	7.896	8.146	8.395	8.647
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.556	2.554	2.551	2.543	2.539	2.534					
18.54	18.60	18.72	23.87	24.39	25.39					
1.000	1.000	1.000	1.000	1.000	1.000					
8.898	9.149	9.400	9.703	9.958	10.218					

182 ITACONIC ACID C5H604

-1	28.0	3.815			130.10		pHL	3.00	3.25	3.50
-2	56.0	5.449					RE	5.643	4.892	4.317
							t	29.41	27.48	26.26
							Z	0.509	0.589	0.670
							pHS	3.771	3.895	4.020

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.820	3.385	3.230	2.959	2.690	2.434	2.377	2.170	1.989	1.827	1.747
25.52	25.25	22.33	22.63	23.28	24.26	27.71	28.80	29.89	28.12	28.66
0.761	0.864	0.915	1.003	1.111	1.237	1.267	1.397	1.536	1.702	1.788
4.161	4.329	4.412	4.563	4.745	4.947	4.996	5.195	5.406	5.691	5.881
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.684	1.640	1.600	1.584	1.574	1.567	1.585	1.582	1.580	1.578	1.580
29.09	29.39	38.42	38.51	38.56	38.58	29.78	29.79	29.81	29.82	29.84
1.861	1.914	1.954	1.972	1.984	1.991	1.995	1.997	1.998	1.999	1.999
6.097	6.331	6.616	6.851	7.094	7.341	7.567	7.815	8.065	8.314	8.565
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 2				
1.579	1.577	1.575	1.565	1.563	1.560					
29.87	29.92	30.01	36.07	36.40	37.03					
2.000	2.000	2.000	2.000	2.000	2.000					
8.815	9.065	9.315	9.587	9.838	10.091					

183 2-KETOGLUTARIC ACID C5H605

-1	33.6	2.800			146.10		pHL	3.00	3.25	3.50
-2	59.0	5.006					RE	2.869	2.675	2.523
							t	27.86	25.63	24.40
							Z	0.849	0.916	0.980
							pHS	3.418	3.590	3.768

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.387	2.251	2.232	2.106	1.972	1.843	1.822	1.718	1.634	1.582	1.548
23.93	24.19	21.77	22.59	23.74	25.02	28.13	29.28	30.23	28.22	28.60
1.048	1.130	1.152	1.247	1.364	1.497	1.517	1.642	1.754	1.850	1.904
3.967	4.184	4.235	4.438	4.652	4.874	4.908	5.123	5.350	5.613	5.832
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.524	1.509	1.491	1.485	1.481	1.477	1.495	1.494	1.492	1.491	1.493
28.86	29.02	37.46	37.51	37.53	37.53	29.20	29.21	29.22	29.23	29.24
1.942	1.966	1.982	1.990	1.994	1.997	1.998	1.999	1.999	2.000	2.000
6.067	6.311	6.588	6.832	7.079	7.328	7.557	7.806	8.056	8.306	8.556
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
1.492	1.490	1.488	1.480	1.478	1.475					
29.27	29.32	29.40	35.11	35.41	35.97					
2.000	2.000	2.000	2.000	2.000	2.000					
8.806	9.057	9.307	9.576	9.827	10.078					

184 LACTIC ACID (S) C3H6O3

-1	36.5	3.860	90.08				pHL	3.00	3.25	3.50
							RE	4.778	4.146	3.673
							t	24.01	22.53	21.53
							Z	0.455	0.526	0.595
							pHS	3.754	3.876	3.996

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.276	2.943	2.830	2.659	2.513	2.403	2.388	2.323	2.281	2.267	2.253
20.77	20.22	17.80	17.58	17.41	17.29	19.65	19.59	19.55	17.37	17.36
0.669	0.747	0.782	0.834	0.884	0.925	0.930	0.957	0.974	0.985	0.991
4.134	4.297	4.379	4.524	4.703	4.913	4.949	5.167	5.402	5.644	5.879
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.243	2.237	2.228	2.225	2.223	2.221	2.235	2.234	2.233	2.231	2.234
17.35	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.123	6.370	6.669	6.917	7.167	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

185 LAURYLSULFONIC ACID C12H26O3S

-1	22.9	1.000	250.40				pHL	3.00	3.25	3.50
							RE	3.641	3.637	3.635
							t	36.88	32.73	30.07
							Z	0.997	0.998	0.999
							pHS	3.439	3.634	3.830

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.633	3.631	3.660	3.658	3.656	3.652	3.642	3.638	3.634	3.665	3.662
28.30	27.19	23.48	22.90	22.53	22.32	26.19	26.07	25.99	22.47	22.45
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
4.043	4.273	4.278	4.497	4.732	4.976	5.013	5.259	5.507	5.729	5.977
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.658	3.654	3.629	3.626	3.623	3.619	3.665	3.663	3.659	3.655	3.662
22.43	22.42	32.74	32.73	32.71	32.70	22.38	22.39	22.40	22.42	22.47
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.226	6.475	6.802	7.052	7.302	7.551	7.726	7.976	8.226	8.476	8.730
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
3.657	3.652	3.646	3.624	3.614	3.600					
22.54	22.68	22.93	30.68	32.02	34.99					
1.000	1.000	1.000	1.000	1.000	1.000					
8.981	9.233	9.486	9.818	10.081	10.357					

186 LEVULINIC ACID C5H8O3

-1	33.4	4.602	116.12				pHL	3.00	3.25	3.50
							RE	9.495	7.988	6.855
							t	24.60	23.30	22.40
							Z	0.247	0.294	0.344
							pHS	4.097	4.200	4.298

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.870	4.991	4.391	3.987	3.586	3.229	3.132	2.906	2.732	2.612	2.553
21.71	21.20	18.47	18.31	18.17	18.06	20.62	20.56	20.52	18.15	18.14
0.403	0.476	0.546	0.603	0.672	0.749	0.772	0.835	0.889	0.937	0.959
4.406	4.533	4.652	4.752	4.882	5.043	5.099	5.270	5.471	5.735	5.932
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.511	2.484	2.458	2.449	2.443	2.439	2.456	2.454	2.452	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.975	0.986	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.157	6.396	6.703	6.945	7.192	7.441	7.638	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 3				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

187 MALEIC ACID C4H404 116.07

-1	41.3	1.921					pHL	3.00	3.25	3.50
-2	62.4	6.225					RE	2.037	2.005	1.984
							t	24.74	22.20	20.64
							Z	0.960	0.976	0.987
							pHS	3.246	3.452	3.662

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.969	1.957	1.964	1.953	1.939	1.919	1.916	1.884	1.837	1.765	1.696
19.69	19.17	17.16	16.96	16.99	17.26	19.45	20.07	21.07	20.73	22.21
0.996	1.005	1.005	1.015	1.029	1.052	1.055	1.094	1.157	1.275	1.386
3.886	4.123	4.132	4.362	4.604	4.851	4.875	5.121	5.368	5.671	5.887
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.624	1.557	1.484	1.452	1.427	1.411	1.418	1.412	1.408	1.405	1.406
23.77	25.22	34.13	34.95	35.54	35.91	28.34	28.46	28.53	28.58	28.61
1.514	1.643	1.783	1.856	1.910	1.947	1.968	1.982	1.990	1.994	1.997
6.108	6.336	6.637	6.850	7.081	7.323	7.557	7.801	8.049	8.298	8.548
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.405	1.403	1.401	1.394	1.392	1.390					
28.65	28.70	28.78	34.15	34.42	34.91					
1.998	1.999	1.999	2.000	2.000	2.000					
8.798	9.048	9.298	9.564	9.815	10.066					

188 MALIC ACID C4H605 134.09

-1	32.6	3.460					pHL	3.00	3.25	3.50
-2	59.0	5.050					RE	3.897	3.436	3.082
							t	27.43	25.72	24.76
							Z	0.640	0.730	0.821
							pHS	3.610	3.748	3.889

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.777	2.508	2.430	2.247	2.068	1.906	1.878	1.755	1.659	1.595	1.557
24.35	24.53	22.12	22.81	23.82	25.01	28.16	29.26	30.19	28.20	28.58
0.921	1.034	1.081	1.188	1.317	1.459	1.482	1.613	1.732	1.838	1.895
4.050	4.236	4.311	4.481	4.676	4.887	4.924	5.133	5.355	5.621	5.836
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.530	1.512	1.492	1.486	1.481	1.478	1.495	1.494	1.492	1.491	1.493
28.85	29.02	37.46	37.51	37.53	37.53	29.20	29.21	29.22	29.23	29.24
1.937	1.963	1.980	1.988	1.993	1.996	1.998	1.999	1.999	2.000	2.000
6.069	6.312	6.589	6.832	7.080	7.329	7.557	7.806	8.056	8.306	8.556
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 7				
1.492	1.490	1.488	1.480	1.478	1.475					
29.27	29.32	29.40	35.11	35.41	35.97					
2.000	2.000	2.000	2.000	2.000	2.000					
8.806	9.057	9.307	9.576	9.827	10.078					

189 MALONIC ACID (S) C3H404 104.06

-1	40.7	2.847					pHL	3.00	3.25	3.50
-2	67.0	5.696					RE	2.489	2.317	2.195
							t	24.10	22.12	20.87
							Z	0.795	0.856	0.907
							pHS	3.384	3.554	3.730

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.102	2.028	2.026	1.971	1.910	1.836	1.824	1.737	1.640	1.528	1.464
20.11	19.78	17.73	17.83	18.29	19.16	21.57	22.89	24.44	24.18	25.23
0.951	0.992	0.998	1.037	1.087	1.157	1.168	1.264	1.386	1.563	1.671
3.928	4.148	4.182	4.394	4.625	4.864	4.897	5.129	5.362	5.664	5.860
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.409	1.367	1.330	1.314	1.303	1.296	1.306	1.304	1.302	1.300	1.301
26.13	26.81	34.51	34.78	34.96	35.05	27.83	27.87	27.89	27.91	27.93
1.772	1.853	1.917	1.949	1.970	1.983	1.990	1.994	1.997	1.998	1.999
6.076	6.308	6.588	6.816	7.058	7.304	7.541	7.788	8.038	8.287	8.538
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.300	1.299	1.298	1.292	1.291	1.289					
27.95	28.00	28.07	33.02	33.25	33.68					
1.999	2.000	2.000	2.000	2.000	2.000					
8.787	9.037	9.288	9.549	9.800	10.051					

190 MANDELIC ACID C8H8O3 152.15

-1	28.3	3.411					pHL	3.00	3.25	3.50
							RE	4.483	4.041	3.715
							t	29.55	27.15	25.53
							Z	0.637	0.709	0.773
							pHS	3.626	3.767	3.912

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.454	3.253	3.241	3.130	3.047	2.991	2.981	2.949	2.928	2.938	2.930
24.36	23.56	20.50	20.13	19.87	19.70	22.80	22.70	22.65	19.82	19.80
0.834	0.887	0.897	0.930	0.956	0.973	0.975	0.986	0.992	0.995	0.997
4.079	4.273	4.315	4.496	4.708	4.938	4.973	5.210	5.454	5.683	5.927

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.925	2.920	2.904	2.902	2.900	2.897	2.925	2.923	2.921	2.918	2.923
19.79	19.79	28.05	28.04	28.03	28.02	19.75	19.75	19.76	19.78	19.80
0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.175	6.424	6.738	6.987	7.237	7.487	7.674	7.924	8.174	8.424	8.676

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 7
2.920	2.917	2.913	2.901	2.896	2.889	
19.85	19.94	20.09	26.06	26.78	28.24	
1.000	1.000	1.000	1.000	1.000	1.000	
8.927	9.178	9.430	9.742	10.000	10.263	

191 MES (S) C6H13NO4S 195.23

-1	28.0	6.095					pHL	3.00	3.25	3.50
							RE	51.093	41.949	35.109
							t	27.00	25.62	24.68
							Z	0.053	0.065	0.078
							pHS	4.838	4.929	5.012

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
29.119	23.671	17.940	15.770	13.471	11.209	9.832	8.414	7.069	4.950	4.581
23.94	23.39	20.11	19.98	19.86	19.77	22.74	22.70	22.68	19.91	19.90
0.094	0.116	0.155	0.177	0.207	0.250	0.286	0.335	0.401	0.584	0.632
5.101	5.201	5.343	5.410	5.495	5.598	5.678	5.776	5.897	6.212	6.300

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
4.177	3.799	3.323	3.200	3.099	3.028	3.021	2.993	2.975	2.963	2.963
19.90	19.90	28.21	28.21	28.22	28.22	19.87	19.87	19.88	19.89	19.92
0.695	0.767	0.878	0.913	0.944	0.966	0.978	0.987	0.993	0.996	0.998
6.422	6.580	6.921	7.083	7.285	7.511	7.711	7.940	8.182	8.429	8.681

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 9
2.957	2.952	2.947	2.934	2.929	2.921	
19.97	20.06	20.22	26.26	27.01	28.51	2-(N-Morpholino)ethane sulfonic
0.999	0.999	1.000	1.000	1.000	1.000	acid
8.930	9.181	9.433	9.746	10.003	10.268	

192 MESACONIC ACID C5H6O4 130.10

-1	28.0	3.098					pHL	3.00	3.25	3.50
-2	56.0	4.750					RE	3.612	3.257	2.968
							t	31.58	29.33	28.16
							Z	0.809	0.902	0.995
							pHS	3.527	3.682	3.843

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.704	2.453	2.392	2.206	2.031	1.884	1.861	1.759	1.684	1.647	1.620
27.76	28.05	25.26	25.94	26.76	27.57	30.94	31.56	32.03	29.40	29.57
1.099	1.220	1.264	1.380	1.510	1.640	1.657	1.762	1.847	1.910	1.945
4.022	4.221	4.288	4.466	4.663	4.876	4.909	5.123	5.351	5.607	5.833

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.602	1.590	1.573	1.569	1.565	1.562	1.582	1.581	1.579	1.577	1.580
29.68	29.75	38.63	38.64	38.63	38.62	29.80	29.81	29.81	29.82	29.84
1.967	1.981	1.990	1.994	1.997	1.998	1.999	1.999	2.000	2.000	2.000
6.072	6.318	6.596	6.842	7.091	7.340	7.565	7.814	8.064	8.314	8.565

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 2
1.578	1.577	1.575	1.565	1.563	1.560	
29.87	29.92	30.02	36.07	36.40	37.03	
2.000	2.000	2.000	2.000	2.000	2.000	
8.815	9.065	9.315	9.587	9.838	10.091	

193 MESOTARTARIC ACID C4H6O6 150.09

-1	32.4	3.222					pHL	3.00	3.25	3.50
-2	60.6	4.815					RE	3.392	3.029	2.743
							t	28.30	26.49	25.57
							Z	0.743	0.839	0.934
							pHS	3.531	3.680	3.835

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.491	2.261	2.201	2.035	1.878	1.743	1.723	1.626	1.555	1.517	1.490
25.32	25.71	23.32	24.10	25.09	26.09	29.16	29.97	30.60	28.35	28.58
1.040	1.162	1.208	1.325	1.459	1.595	1.614	1.728	1.822	1.895	1.935
4.009	4.205	4.275	4.453	4.651	4.865	4.898	5.110	5.338	5.598	5.822
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.472	1.461	1.446	1.442	1.438	1.435	1.452	1.451	1.449	1.448	1.450
28.74	28.83	37.00	37.02	37.02	37.02	28.91	28.92	28.93	28.94	28.95
1.961	1.978	1.988	1.993	1.996	1.998	1.999	1.999	2.000	2.000	2.000
6.060	6.306	6.579	6.825	7.073	7.322	7.552	7.802	8.052	8.302	8.552
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
1.449	1.448	1.446	1.438	1.436	1.434					
28.98	29.02	29.11	34.64	34.93	35.45					
2.000	2.000	2.000	2.000	2.000	2.000					
8.802	9.052	9.303	9.570	9.821	10.072					

194 METHACRYLIC ACID C4H6O2 86.09

-1	36.7	4.483					pHL	3.00	3.25	3.50
							RE	7.858	6.634	5.716
							t	23.20	22.03	21.22
							Z	0.272	0.323	0.375
							pHS	4.033	4.137	4.237

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.918	4.208	3.738	3.411	3.089	2.808	2.739	2.561	2.427	2.340	2.295
20.59	20.12	17.64	17.49	17.36	17.25	19.58	19.52	19.49	17.33	17.32
0.438	0.513	0.583	0.640	0.709	0.782	0.802	0.859	0.908	0.948	0.967
4.347	4.478	4.597	4.701	4.835	5.002	5.055	5.232	5.439	5.702	5.905
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.263	2.243	2.224	2.218	2.214	2.210	2.224	2.222	2.221	2.219	2.221
17.31	17.31	23.59	23.59	23.59	23.58	17.27	17.28	17.28	17.29	17.30
0.980	0.988	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.134	6.375	6.676	6.919	7.166	7.415	7.619	7.868	8.118	8.368	8.619
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
2.220	2.218	2.216	2.211	2.208	2.205					
17.33	17.39	17.48	21.89	22.26	22.97					
1.000	1.000	1.000	1.000	1.000	1.000					
8.869	9.120	9.371	9.664	9.918	10.174					

195 METHOXYACETIC ACID C3H6O3 90.08

-1	36.5	3.570					pHL	3.00	3.25	3.50
							RE	3.934	3.478	3.139
							t	24.46	22.79	21.66
							Z	0.556	0.630	0.700
							pHS	3.637	3.770	3.905

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.863	2.642	2.597	2.480	2.387	2.323	2.315	2.277	2.254	2.252	2.244
20.83	20.24	17.86	17.60	17.41	17.29	19.65	19.59	19.55	17.37	17.36
0.769	0.836	0.855	0.896	0.932	0.958	0.961	0.977	0.987	0.992	0.995
4.059	4.241	4.303	4.469	4.669	4.893	4.923	5.154	5.395	5.633	5.874
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.238	2.234	2.226	2.224	2.223	2.221	2.235	2.234	2.233	2.231	2.234
17.35	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.121	6.369	6.668	6.917	7.166	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 7				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

196 m-METHOXYBENZOIC ACID C8H8O3
-1 28.3 4.088 152.15

pHL	3.00	3.25	3.50
RE	7.060	6.077	5.335
t	28.31	26.42	25.13
Z	0.399	0.465	0.531
pHS	3.885	4.001	4.115

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.701	4.159	3.961	3.682	3.433	3.240	3.205	3.088	3.011	2.986	2.959
24.17	23.48	20.33	20.06	19.85	19.70	22.77	22.69	22.64	19.82	19.80
0.605	0.687	0.727	0.784	0.843	0.895	0.904	0.939	0.963	0.978	0.987
4.245	4.398	4.482	4.615	4.784	4.984	5.028	5.239	5.469	5.707	5.937
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.941	2.929	2.909	2.905	2.901	2.898	2.925	2.923	2.921	2.918	2.923
19.79	19.79	28.05	28.04	28.03	28.02	19.75	19.75	19.76	19.78	19.80
0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.179	6.426	6.741	6.988	7.237	7.487	7.674	7.924	8.174	8.424	8.676
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.920	2.917	2.913	2.901	2.896	2.889					
19.85	19.94	20.09	26.06	26.78	28.24					
1.000	1.000	1.000	1.000	1.000	1.000					
8.927	9.178	9.430	9.742	10.000	10.263					

197 o-METHOXYBENZOIC ACID C8H8O3
-1 28.3 4.094 152.15

pHL	3.00	3.25	3.50
RE	7.093	6.103	5.356
t	28.30	26.41	25.13
Z	0.397	0.463	0.529
pHS	3.888	4.003	4.117

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.718	4.173	3.971	3.690	3.439	3.244	3.208	3.091	3.013	2.986	2.959
24.17	23.48	20.32	20.06	19.85	19.70	22.77	22.69	22.64	19.82	19.80
0.603	0.684	0.725	0.783	0.842	0.894	0.903	0.938	0.963	0.978	0.987
4.246	4.400	4.483	4.617	4.785	4.984	5.029	5.240	5.470	5.708	5.938
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.941	2.929	2.909	2.905	2.901	2.898	2.925	2.923	2.921	2.918	2.923
19.79	19.79	28.05	28.04	28.03	28.02	19.75	19.75	19.76	19.78	19.80
0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
6.179	6.426	6.741	6.988	7.237	7.487	7.674	7.924	8.174	8.424	8.676
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.920	2.917	2.913	2.901	2.896	2.889					
19.85	19.94	20.09	26.06	26.78	28.24					
1.000	1.000	1.000	1.000	1.000	1.000					
8.927	9.178	9.430	9.742	10.000	10.263					

198 p-METHOXYBENZOIC ACID C8H8O3
-1 30.0 4.471 152.15

pHL	3.00	3.25	3.50
RE	9.253	7.823	6.745
t	26.64	25.07	24.01
Z	0.284	0.337	0.392
pHS	4.048	4.154	4.256

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.810	4.985	4.511	4.114	3.731	3.403	3.324	3.118	2.967	2.880	2.829
23.20	22.60	19.58	19.38	19.21	19.08	21.95	21.89	21.85	19.19	19.18
0.456	0.534	0.596	0.656	0.725	0.797	0.816	0.872	0.917	0.952	0.970
4.369	4.503	4.610	4.719	4.859	5.032	5.085	5.269	5.480	5.733	5.942
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.793	2.770	2.744	2.737	2.732	2.727	2.751	2.749	2.746	2.744	2.747
19.17	19.17	26.93	26.93	26.92	26.91	19.13	19.13	19.14	19.15	19.18
0.982	0.990	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.174	6.416	6.729	6.973	7.221	7.470	7.661	7.911	8.160	8.410	8.663
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.745	2.742	2.739	2.729	2.725	2.719					
19.22	19.30	19.43	25.00	25.62	26.84					
1.000	1.000	1.000	1.000	1.000	1.000					
8.913	9.164	9.416	9.723	9.980	10.242					

199 p-METHOXYPHENYLACETIC ACID C9H1003 166.18

-1	29.7	4.361					pHL	3.00	3.25	3.50
							RE	8.480	7.200	6.235
							t	26.96	25.33	24.21
							Z	0.314	0.371	0.429
							pHS	3.999	4.108	4.213

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.402	4.671	4.293	3.934	3.595	3.312	3.249	3.074	2.948	2.884	2.841
23.37	22.75	19.71	19.50	19.32	19.18	22.10	22.03	21.98	19.30	19.28
0.497	0.578	0.635	0.694	0.762	0.829	0.845	0.895	0.934	0.962	0.976
4.330	4.469	4.570	4.685	4.833	5.013	5.064	5.256	5.473	5.721	5.938
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.812	2.793	2.770	2.764	2.760	2.756	2.780	2.778	2.776	2.773	2.777
19.27	19.27	27.12	27.11	27.11	27.10	19.23	19.24	19.24	19.26	19.28
0.986	0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.173	6.417	6.730	6.976	7.224	7.473	7.663	7.913	8.163	8.413	8.665
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
2.774	2.772	2.768	2.758	2.753	2.747					
19.33	19.40	19.54	25.18	25.81	27.07					
1.000	1.000	1.000	1.000	1.000	1.000					
8.915	9.166	9.418	9.727	9.983	10.245					

200 METHYLETHYLMALONIC ACID C6H1004 146.14

-1	25.0	2.860					pHL	3.00	3.25	3.50
-2	50.0	6.413					RE	3.954	3.743	3.593
							t	33.54	30.28	28.13
							Z	0.831	0.879	0.917
							pHS	3.514	3.680	3.853

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.479	3.393	3.411	3.352	3.292	3.221	3.201	3.103	2.965	2.745	2.566
26.66	25.76	22.34	21.96	21.83	21.97	25.57	26.03	26.81	25.10	26.23
0.949	0.974	0.976	0.994	1.013	1.036	1.041	1.076	1.129	1.240	1.336
4.048	4.265	4.285	4.492	4.721	4.960	5.001	5.241	5.480	5.796	5.994
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.380	2.207	2.001	1.925	1.864	1.821	1.825	1.809	1.799	1.791	1.792
27.40	28.50	39.61	40.12	40.52	40.77	31.00	31.10	31.16	31.21	31.25
1.451	1.576	1.743	1.819	1.882	1.928	1.956	1.974	1.985	1.992	1.995
6.199	6.412	6.740	6.930	7.148	7.382	7.605	7.842	8.087	8.335	8.586
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2				
1.788	1.785	1.782	1.769	1.766	1.761					
31.30	31.36	31.48	38.37	38.80	39.61					
1.997	1.998	1.999	2.000	2.000	2.000					
8.835	9.085	9.335	9.614	9.866	10.119					

201 METHYLMALONIC ACID C4H604 118.09

-1	29.3	3.072					pHL	3.00	3.25	3.50
-2	58.5	5.787					RE	3.665	3.384	3.177
							t	29.59	27.03	25.36
							Z	0.757	0.822	0.877
							pHS	3.518	3.675	3.839

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.010	2.871	2.866	2.758	2.636	2.491	2.459	2.293	2.114	1.901	1.793
24.28	23.72	20.84	20.82	21.18	21.92	25.13	26.22	27.48	26.38	27.17
0.928	0.975	0.983	1.024	1.075	1.142	1.157	1.248	1.362	1.545	1.647
4.024	4.234	4.273	4.474	4.696	4.929	4.974	5.197	5.421	5.730	5.911
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.698	1.626	1.559	1.533	1.514	1.502	1.515	1.511	1.508	1.506	1.507
27.87	28.41	37.24	37.43	37.55	37.62	29.25	29.28	29.29	29.31	29.33
1.748	1.833	1.907	1.942	1.966	1.980	1.988	1.993	1.996	1.998	1.999
6.116	6.339	6.632	6.852	7.089	7.334	7.563	7.810	8.058	8.308	8.558
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
1.506	1.504	1.502	1.494	1.491	1.489					
29.36	29.41	29.50	35.26	35.57	36.14					
1.999	2.000	2.000	2.000	2.000	2.000					
8.808	9.058	9.308	9.578	9.829	10.080					

202 METHYLSULFONIC ACID CH4O3S

-1	50.6	-2.000	96.10

pHL	3.00	3.25	3.50
RE	1.584	1.584	1.584
t	22.29	19.92	18.52
Z	1.000	1.000	1.000
pHS	3.145	3.371	3.598

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.584	1.583	1.587	1.587	1.586	1.586	1.585	1.585	1.584	1.588	1.587
17.67	17.17	15.57	15.29	15.13	15.04	16.72	16.68	16.65	15.10	15.09
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.834	4.077	4.079	4.317	4.562	4.810	4.823	5.072	5.321	5.561	5.811
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.587	1.586	1.584	1.584	1.583	1.583	1.588	1.587	1.587	1.586	1.587
15.09	15.09	19.58	19.58	19.58	19.58	15.06	15.06	15.06	15.07	15.08
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.060	6.310	6.587	6.837	7.087	7.337	7.560	7.810	8.060	8.310	8.561
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.587	1.586	1.585	1.584	1.583	1.582					
15.09	15.12	15.17	18.26	18.45	18.78					
1.000	1.000	1.000	1.000	1.000	1.000					
8.811	9.061	9.312	9.584	9.836	10.089					

203 2-NAPHTALENESULFONIC ACID C10H8O3S

-1	31.3	0.167	208.23

pHL	3.00	3.25	3.50
RE	2.614	2.613	2.613
t	29.64	26.35	24.30
Z	0.999	1.000	1.000
pHS	3.318	3.523	3.730

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.612	2.611	2.626	2.625	2.624	2.621	2.618	2.616	2.613	2.628	2.627
22.99	22.18	19.51	19.08	18.82	18.67	21.45	21.37	21.32	18.77	18.75
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.951	4.186	4.190	4.416	4.656	4.901	4.929	5.175	5.424	5.653	5.901
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.625	2.623	2.612	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.400	6.708	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 2				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

204 NICOTINIC ACID C6H5NO2

1	34.6	2.070	123.11
-1	-34.6	4.819	

pHL	3.00	3.25	3.50
RE	11.277	9.448	8.068
t	24.32	23.01	22.10
Z	0.200	0.239	0.280
pHS	4.216	4.309	4.398

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.856	5.763	4.887	4.408	3.920	3.468	3.318	3.028	2.791	2.596	2.517
21.38	20.84	18.16	18.01	17.87	17.76	20.21	20.16	20.12	17.83	17.82
0.331	0.395	0.471	0.523	0.590	0.669	0.700	0.770	0.837	0.907	0.936
4.497	4.614	4.743	4.832	4.948	5.094	5.156	5.309	5.495	5.771	5.949
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.456	2.415	2.379	2.367	2.359	2.353	2.368	2.365	2.363	2.361	2.364
17.81	17.81	24.49	24.49	24.49	24.48	17.77	17.78	17.78	17.79	17.81
0.960	0.976	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.162	6.394	6.702	6.939	7.184	7.432	7.632	7.880	8.130	8.380	8.631
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
2.362	2.360	2.357	2.351	2.348	2.344					
17.84	17.90	18.00	22.72	23.15	23.97					
1.000	1.000	1.000	1.000	1.000	1.000					
8.882	9.132	9.383	9.680	9.935	10.193					

205 NITRIC ACID HNO3

-1	74.1	-1.370	63.01				pHL	3.00	3.25	3.50
							RE	1.069	1.069	1.069
							t	18.57	16.69	15.63
							Z	1.000	1.000	1.000
							pHS	3.020	3.267	3.513

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069
15.03	14.69	13.62	13.43	13.32	13.26	14.39	14.36	14.34	13.29	13.29
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.761	4.010	4.010	4.259	4.508	4.758	4.759	5.009	5.259	5.508	5.758

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069	1.069
13.29	13.29	16.31	16.31	16.31	16.31	13.26	13.27	13.27	13.28	13.28
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.008	6.258	6.511	6.761	7.011	7.261	7.507	7.758	8.008	8.258	8.508

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 2
1.069	1.069	1.069	1.069	1.069	1.069	
13.29	13.30	13.33	15.38	15.47	15.63	
1.000	1.000	1.000	1.000	1.000	1.000	
8.758	9.008	9.258	9.511	9.761	10.011	

206 2-NITRO-3-BROMOBENZOIC ACID C7H4BrNO4

-1	28.2	2.495	246.02				pHL	3.00	3.25	3.50
							RE	3.222	3.116	3.045
							t	31.18	27.99	25.92
							Z	0.901	0.933	0.955
							pHS	3.421	3.603	3.790

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.995	2.961	2.979	2.960	2.946	2.936	2.931	2.924	2.919	2.937	2.935
24.53	23.65	20.66	20.20	19.92	19.74	22.85	22.76	22.70	19.86	19.84
0.972	0.983	0.984	0.990	0.994	0.997	0.997	0.998	0.999	0.999	1.000
3.996	4.222	4.234	4.450	4.684	4.927	4.958	5.203	5.451	5.677	5.925

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.932	2.929	2.914	2.913	2.910	2.907	2.936	2.934	2.932	2.929	2.934
19.83	19.83	28.12	28.11	28.10	28.09	19.79	19.79	19.80	19.82	19.84
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.175	6.424	6.738	6.988	7.238	7.488	7.674	7.924	8.174	8.425	8.677

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.931	2.928	2.924	2.912	2.907	2.899	
19.89	19.98	20.13	26.13	26.86	28.33	
1.000	1.000	1.000	1.000	1.000	1.000	
8.928	9.179	9.431	9.744	10.001	10.265	

207 3-NITRO-2-BROMOBENZOIC ACID C7H4BrNO4

-1	28.2	2.979	246.02				pHL	3.00	3.25	3.50
							RE	3.686	3.445	3.274
							t	30.47	27.66	25.79
							Z	0.784	0.840	0.886
							pHS	3.506	3.667	3.835

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.145	3.054	3.066	3.015	2.979	2.955	2.949	2.934	2.925	2.941	2.937
24.49	23.64	20.62	20.19	19.91	19.74	22.85	22.76	22.70	19.86	19.84
0.923	0.952	0.954	0.971	0.982	0.990	0.991	0.995	0.997	0.998	0.999
4.025	4.239	4.261	4.464	4.691	4.930	4.963	5.205	5.452	5.679	5.926

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.933	2.929	2.915	2.913	2.910	2.908	2.936	2.934	2.932	2.929	2.934
19.83	19.83	28.12	28.11	28.10	28.09	19.79	19.79	19.80	19.82	19.84
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.175	6.424	6.739	6.988	7.238	7.488	7.674	7.924	8.174	8.425	8.677

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3
2.931	2.928	2.924	2.912	2.907	2.899	
19.89	19.98	20.13	26.13	26.86	28.33	
1.000	1.000	1.000	1.000	1.000	1.000	
8.928	9.179	9.431	9.744	10.001	10.265	

208 3-NITRO-4-BROMOBENZOIC ACID C7H4BrNO4

-1	28.2	3.377	246.02				pHL	3.00	3.25	3.50
							RE	4.415	3.991	3.679
							t	29.70	27.25	25.61
							Z	0.650	0.721	0.784
							pHS	3.616	3.758	3.905

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.431	3.241	3.232	3.127	3.049	2.997	2.987	2.957	2.937	2.948	2.941
24.42	23.62	20.55	20.17	19.91	19.74	22.85	22.75	22.70	19.86	19.84
0.843	0.894	0.903	0.934	0.959	0.975	0.977	0.987	0.992	0.995	0.997
4.074	4.270	4.310	4.493	4.706	4.938	4.973	5.210	5.454	5.683	5.928
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.935	2.931	2.915	2.913	2.911	2.908	2.936	2.934	2.932	2.929	2.934
19.83	19.83	28.12	28.11	28.10	28.09	19.79	19.79	19.80	19.82	19.84
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.175	6.425	6.739	6.988	7.238	7.488	7.675	7.924	8.174	8.425	8.677
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.931	2.928	2.924	2.912	2.907	2.899					
19.89	19.98	20.13	26.13	26.86	28.33					
1.000	1.000	1.000	1.000	1.000	1.000					
8.928	9.179	9.431	9.744	10.001	10.265					

209 2-NITRO-3-CHLOROBENZOIC ACID C7H4ClNO4

-1	31.3	2.398	201.57				pHL	3.00	3.25	3.50
							RE	2.857	2.771	2.714
							t	29.10	26.14	24.23
							Z	0.912	0.941	0.961
							pHS	3.377	3.563	3.755

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.674	2.648	2.662	2.646	2.636	2.628	2.625	2.619	2.615	2.630	2.628
22.97	22.17	19.49	19.08	18.82	18.67	21.45	21.37	21.32	18.77	18.75
0.976	0.986	0.986	0.991	0.995	0.997	0.997	0.998	0.999	0.999	1.000
3.965	4.194	4.204	4.423	4.659	4.903	4.931	5.176	5.425	5.654	5.902
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.625	2.623	2.612	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.708	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

210 3-NITRO-4-CHLOROBENZOIC ACID C7H4ClNO4

-1	31.3	3.357	201.57				pHL	3.00	3.25	3.50
							RE	3.983	3.595	3.309
							t	27.58	25.40	23.92
							Z	0.646	0.718	0.782
							pHS	3.588	3.731	3.879

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.082	2.909	2.897	2.802	2.732	2.685	2.677	2.650	2.633	2.640	2.634
22.86	22.14	19.39	19.05	18.81	18.67	21.45	21.36	21.31	18.77	18.75
0.841	0.893	0.902	0.934	0.958	0.975	0.977	0.987	0.992	0.995	0.997
4.048	4.244	4.286	4.470	4.683	4.915	4.946	5.184	5.428	5.660	5.904
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.629	2.625	2.613	2.612	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.152	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

211 3-NITRO-5-CHLOROBENZOIC ACID C7H4ClNO4

-1	31.3	3.130	201.57							
							pHL	3.00	3.25	3.50
							RE	3.564	3.277	3.070
							t	28.01	25.62	24.03
							Z	0.725	0.790	0.845
							pHS	3.519	3.673	3.833

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.912	2.796	2.799	2.735	2.689	2.659	2.654	2.636	2.625	2.635	2.631
22.90	22.15	19.43	19.06	18.82	18.67	21.45	21.36	21.31	18.77	18.75
0.893	0.931	0.935	0.958	0.974	0.985	0.986	0.992	0.995	0.997	0.998
4.015	4.223	4.254	4.450	4.672	4.909	4.939	5.180	5.427	5.657	5.903
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.627	2.624	2.613	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

212 m-NITROBENZOIC ACID C7H5NO4

-1	32.3	3.493	167.12							
							pHL	3.00	3.25	3.50
							RE	4.182	3.730	3.395
							t	26.73	24.73	23.38
							Z	0.594	0.668	0.736
							pHS	3.629	3.766	3.906

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.125	2.913	2.884	2.769	2.680	2.620	2.611	2.576	2.554	2.558	2.550
22.40	21.72	19.04	18.73	18.51	18.36	21.05	20.97	20.93	18.46	18.45
0.802	0.862	0.876	0.913	0.944	0.966	0.969	0.981	0.989	0.994	0.996
4.066	4.254	4.306	4.480	4.686	4.913	4.945	5.179	5.422	5.656	5.898
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.544	2.540	2.529	2.527	2.525	2.523	2.543	2.542	2.540	2.537	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.146	6.394	6.700	6.950	7.199	7.449	7.644	7.894	8.144	8.394	8.646
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1				
2.539	2.537	2.534	2.526	2.523	2.518					
18.48	18.54	18.66	23.77	24.28	25.27					
1.000	1.000	1.000	1.000	1.000	1.000					
8.896	9.147	9.399	9.701	9.956	10.215					

213 o-NITROBENZOIC ACID C7H5NO4

-1	33.6	2.173	167.12							
							pHL	3.00	3.25	3.50
							RE	2.575	2.521	2.486
							t	27.94	25.04	23.20
							Z	0.940	0.961	0.975
							pHS	3.332	3.526	3.725

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.461	2.446	2.457	2.448	2.442	2.437	2.434	2.430	2.427	2.439	2.438
22.00	21.26	18.78	18.39	18.14	18.00	20.59	20.51	20.46	18.10	18.08
0.985	0.991	0.991	0.995	0.997	0.998	0.998	0.999	0.999	1.000	1.000
3.941	4.173	4.181	4.404	4.642	4.887	4.912	5.159	5.407	5.638	5.886
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.436	2.434	2.425	2.424	2.423	2.421	2.439	2.438	2.436	2.434	2.437
18.07	18.07	24.97	24.96	24.96	24.95	18.03	18.04	18.04	18.06	18.07
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.136	6.385	6.689	6.938	7.188	7.438	7.636	7.886	8.136	8.386	8.637
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.436	2.433	2.431	2.424	2.421	2.417					
18.11	18.17	18.28	23.16	23.62	24.51					
1.000	1.000	1.000	1.000	1.000	1.000					
8.888	9.138	9.390	9.689	9.944	10.202					

214 p-NITROBENZOIC ACID C7H5NO4

-1 32.3 3.523 167.12

pHL	3.00	3.25	3.50
RE	4.257	3.788	3.441
t	26.67	24.70	23.37
Z	0.583	0.657	0.726
pHS	3.640	3.775	3.913

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.158	2.936	2.903	2.783	2.690	2.626	2.617	2.580	2.556	2.559	2.551
22.39	21.72	19.03	18.73	18.50	18.36	21.05	20.97	20.93	18.46	18.45
0.793	0.855	0.870	0.909	0.941	0.964	0.967	0.980	0.989	0.993	0.996
4.072	4.258	4.312	4.484	4.688	4.914	4.947	5.180	5.423	5.656	5.899

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.545	2.540	2.529	2.527	2.525	2.523	2.543	2.542	2.540	2.537	2.541
18.44	18.44	25.62	25.62	25.61	25.61	18.40	18.40	18.41	18.42	18.44
0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.146	6.394	6.700	6.950	7.199	7.449	7.644	7.894	8.144	8.394	8.646

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1
2.539	2.537	2.534	2.526	2.523	2.518	
18.48	18.54	18.66	23.77	24.28	25.27	
1.000	1.000	1.000	1.000	1.000	1.000	
8.896	9.147	9.399	9.701	9.956	10.215	

215 m-NITROPHENOL C6H5NO3

-1 33.4 8.399 139.11

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	□□□□□□
t	23.80	22.79	22.09
Z	0.004	0.005	0.005
pHS	5.973	6.060	6.138

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	95.764	80.705	65.677	30.949	28.181
21.54	21.10	18.36	18.28	18.19	18.12	20.53	20.50	20.48	18.21	18.21
0.007	0.008	0.012	0.014	0.016	0.019	0.024	0.028	0.035	0.074	0.081
6.221	6.314	6.474	6.530	6.602	6.690	6.777	6.853	6.945	7.291	7.335

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
24.723	20.887	10.255	9.451	8.430	7.285	4.914	4.555	4.128	3.689	3.161
18.21	18.21	24.87	24.88	24.89	24.90	18.16	18.16	18.16	18.17	18.19
0.093	0.110	0.227	0.247	0.278	0.322	0.486	0.525	0.581	0.653	0.767
7.397	7.478	7.849	7.896	7.964	8.054	8.347	8.414	8.511	8.641	8.883

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1
2.951	2.773	2.643	2.541	2.494	2.464	
18.22	18.28	18.39	23.31	23.78	24.69	
0.824	0.878	0.922	0.958	0.975	0.986	
9.033	9.220	9.435	9.723	9.961	10.213	

216 o-NITROPHENOL C6H5NO3

-1 33.4 7.234 139.11

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	□□□□□□
t	23.81	22.79	22.09
Z	0.014	0.017	0.021
pHS	5.391	5.479	5.558

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
89.568	72.459	51.238	45.044	38.317	31.525	26.323	22.272	18.254	9.625	8.802
21.52	21.09	18.34	18.25	18.16	18.09	20.52	20.49	20.47	18.17	18.17
0.025	0.031	0.045	0.051	0.060	0.073	0.087	0.103	0.126	0.244	0.267
5.641	5.736	5.893	5.952	6.026	6.116	6.202	6.282	6.379	6.722	6.774

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
7.792	6.700	4.268	3.979	3.640	3.300	2.928	2.798	2.678	2.588	2.531
18.17	18.16	24.95	24.96	24.97	24.99	18.10	18.10	18.11	18.12	18.13
0.302	0.352	0.560	0.601	0.659	0.729	0.832	0.872	0.912	0.944	0.968
6.848	6.946	7.310	7.384	7.490	7.632	7.892	8.030	8.211	8.424	8.673

8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 1
2.497	2.475	2.461	2.447	2.440	2.434	
18.17	18.23	18.34	23.25	23.72	24.62	
0.981	0.989	0.994	0.997	0.998	0.999	
8.904	9.147	9.395	9.693	9.946	10.205	

217 p-NITROPHENOL C6H5NO3

-1 33.4 7.149 139.11

pHL	3.00	3.25	3.50
RE	□□□□□□	□□□□□□	98.291
t	23.81	22.80	22.09
Z	0.016	0.019	0.023
pHS	5.349	5.436	5.515

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
81.358	65.835	46.641	41.010	34.896	28.725	24.031	20.344	16.691	8.923	8.165
21.52	21.09	18.34	18.25	18.16	18.09	20.52	20.49	20.47	18.17	18.17
0.028	0.034	0.049	0.056	0.066	0.080	0.096	0.113	0.138	0.263	0.288
5.599	5.694	5.851	5.910	5.984	6.075	6.161	6.241	6.339	6.681	6.734

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
7.237	6.238	4.073	3.803	3.490	3.182	2.867	2.748	2.643	2.565	2.518
18.16	18.16	24.96	24.97	24.98	24.99	18.10	18.10	18.11	18.12	18.13
0.326	0.379	0.587	0.630	0.688	0.757	0.850	0.888	0.925	0.953	0.973
6.810	6.910	7.273	7.351	7.462	7.611	7.867	8.012	8.200	8.418	8.668

8.75	9.00	9.25	9.50	9.75	10.00
2.489	2.470	2.458	2.445	2.439	2.434
18.17	18.23	18.34	23.25	23.72	24.62
0.984	0.991	0.995	0.997	0.999	0.999
8.902	9.146	9.394	9.693	9.946	10.205

(Ref.) : 3 , 1

218 NITROUS ACID HNO2

-1 74.6 3.220 47.01

pHL	3.00	3.25	3.50
RE	1.684	1.501	1.370
t	16.80	15.94	15.36
Z	0.625	0.702	0.770
pHS	3.404	3.554	3.706

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.268	1.192	1.175	1.136	1.107	1.088	1.087	1.077	1.070	1.067	1.065
14.94	14.65	13.52	13.39	13.29	13.24	14.36	14.33	14.31	13.27	13.26
0.833	0.888	0.901	0.933	0.958	0.975	0.976	0.986	0.992	0.995	0.997
3.878	4.076	4.138	4.324	4.539	4.772	4.782	5.019	5.263	5.516	5.760

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.063	1.063	1.062	1.062	1.062	1.062	1.062	1.062	1.062	1.062	1.062
13.26	13.26	16.26	16.26	16.27	16.27	13.24	13.24	13.25	13.25	13.25
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.008	6.257	6.511	6.761	7.010	7.260	7.507	7.757	8.007	8.257	8.507

8.75	9.00	9.25	9.50	9.75	10.00
1.062	1.062	1.062	1.062	1.062	1.062
13.26	13.28	13.31	15.34	15.43	15.58
1.000	1.000	1.000	1.000	1.000	1.000
8.757	9.007	9.257	9.510	9.760	10.010

(Ref.) : 2 , 7

219 OCTYLSULFONIC ACID C8H1803S

-1 30.1 -2.000 194.30

pHL	3.00	3.25	3.50
RE	2.722	2.722	2.722
t	30.42	27.04	24.92
Z	1.000	1.000	1.000
pHS	3.332	3.536	3.742

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.721	2.720	2.736	2.736	2.734	2.732	2.728	2.725	2.723	2.739	2.738
23.55	22.71	19.94	19.49	19.22	19.06	21.96	21.87	21.82	19.16	19.15
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.962	4.196	4.200	4.426	4.664	4.910	4.938	5.185	5.434	5.662	5.910

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.736	2.733	2.722	2.720	2.718	2.715	2.740	2.738	2.736	2.734	2.738
19.14	19.13	26.87	26.87	26.86	26.85	19.09	19.10	19.11	19.12	19.14
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.159	6.409	6.720	6.969	7.219	7.469	7.659	7.909	8.159	8.409	8.662

8.75	9.00	9.25	9.50	9.75	10.00
2.735	2.733	2.729	2.720	2.715	2.709
19.18	19.26	19.40	24.94	25.56	26.77
1.000	1.000	1.000	1.000	1.000	1.000
8.912	9.163	9.415	9.722	9.979	10.240

(Ref.) : 3 , 12

220 OROTIC ACID C5H4N2O4

-1	33.1	2.803	156.10				pHL	3.00	3.25	3.50
							RE	2.988	2.817	2.697
							t	27.50	24.97	23.31
							Z	0.819	0.870	0.910
							pHS	3.425	3.595	3.773

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.611	2.551	2.560	2.527	2.504	2.489	2.485	2.476	2.470	2.481	2.478
22.17	21.44	18.89	18.52	18.28	18.14	20.76	20.68	20.64	18.23	18.22
0.941	0.964	0.965	0.978	0.987	0.993	0.993	0.996	0.998	0.999	0.999
3.971	4.191	4.210	4.421	4.652	4.893	4.920	5.164	5.412	5.643	5.890
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.476	2.473	2.464	2.463	2.461	2.459	2.478	2.477	2.475	2.473	2.476
18.21	18.21	25.21	25.21	25.20	25.20	18.17	18.17	18.18	18.19	18.21
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.139	6.389	6.693	6.943	7.192	7.442	7.639	7.889	8.139	8.389	8.641
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
2.474	2.472	2.469	2.462	2.459	2.455					
18.25	18.31	18.42	23.39	23.87	24.79					
1.000	1.000	1.000	1.000	1.000	1.000					
8.891	9.142	9.393	9.693	9.948	10.207					

221 OXALIC ACID (S) C2H2O4

-1	42.4	1.271	90.04				pHL	3.00	3.25	3.50
-2	77.0	4.266					RE	1.785	1.709	1.619
							t	26.36	24.63	24.23
							Z	1.095	1.159	1.244
							pHS	3.213	3.434	3.651

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.517	1.414	1.397	1.318	1.252	1.203	1.198	1.166	1.145	1.137	1.130
24.63	25.43	23.55	24.31	25.00	25.54	27.88	28.25	28.50	26.52	26.61
1.353	1.481	1.513	1.629	1.738	1.828	1.832	1.895	1.937	1.964	1.979
3.871	4.094	4.146	4.348	4.564	4.794	4.808	5.040	5.280	5.535	5.775
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.126	1.123	1.116	1.115	1.114	1.112	1.121	1.121	1.120	1.120	1.121
26.66	26.69	32.97	32.98	32.98	32.97	26.68	26.69	26.70	26.71	26.71
1.988	1.993	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000
6.021	6.270	6.527	6.775	7.025	7.274	7.519	7.769	8.019	8.269	8.519
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.120	1.120	1.119	1.115	1.114	1.113					
26.73	26.76	26.82	31.07	31.25	31.57					
2.000	2.000	2.000	2.000	2.000	2.000					
8.769	9.019	9.269	9.524	9.774	10.024					

222 OXALOACETIC ACID C4H4O5

-1	28.0	2.555	132.07				pHL	3.00	3.25	3.50
-2	56.0	4.370					RE	2.924	2.698	2.492
							t	33.32	30.94	29.88
							Z	1.011	1.102	1.200
							pHS	3.414	3.593	3.775

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.291	2.100	2.069	1.932	1.816	1.727	1.715	1.658	1.620	1.611	1.597
29.68	30.04	27.15	27.67	28.21	28.66	31.99	32.30	32.50	29.67	29.74
1.315	1.446	1.482	1.597	1.710	1.806	1.814	1.882	1.928	1.959	1.976
3.969	4.176	4.231	4.417	4.624	4.848	4.872	5.099	5.337	5.585	5.822
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.588	1.582	1.569	1.566	1.564	1.561	1.581	1.580	1.579	1.577	1.580
29.78	29.81	38.66	38.66	38.64	38.62	29.81	29.81	29.81	29.82	29.84
1.986	1.992	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000
6.068	6.316	6.593	6.841	7.090	7.340	7.564	7.814	8.064	8.314	8.565
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 1				
1.578	1.577	1.575	1.565	1.563	1.560					
29.87	29.92	30.02	36.07	36.40	37.03					
2.000	2.000	2.000	2.000	2.000	2.000					
8.815	9.065	9.315	9.587	9.838	10.091					

223 PELARGONIC ACID C9H18O2

-1	26.7	4.955			158.24		pHL	3.00	3.25	3.50
							RE	16.050	13.381	11.369
							t	28.51	26.84	25.71
							Z	0.182	0.219	0.259
							pHS	4.287	4.386	4.479

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
9.613	8.038	6.880	6.160	5.433	4.766	4.534	4.103	3.750	3.467	3.347
24.85	24.22	20.79	20.61	20.45	20.32	23.54	23.49	23.45	20.47	20.46
0.307	0.369	0.436	0.489	0.557	0.637	0.671	0.744	0.816	0.892	0.925
4.582	4.700	4.819	4.909	5.026	5.170	5.234	5.386	5.569	5.838	6.013
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.253	3.189	3.128	3.108	3.095	3.087	3.116	3.113	3.108	3.105	3.109
20.45	20.45	29.22	29.22	29.21	29.20	20.41	20.42	20.42	20.44	20.47
0.953	0.972	0.986	0.992	0.995	0.997	0.998	0.999	0.999	1.000	1.000
6.223	6.454	6.776	7.013	7.258	7.505	7.690	7.938	8.188	8.438	8.691
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 7				
3.106	3.102	3.098	3.084	3.078	3.069					
20.53	20.62	20.80	27.20	28.05	29.79					
1.000	1.000	1.000	1.000	1.000	1.000					
8.941	9.192	9.444	9.762	10.020	10.287					

224 PERCHLORIC ACID (S) HClO4

-1	69.8	-2.000			100.46		pHL	3.00	3.25	3.50
							RE	1.137	1.137	1.137
							t	19.06	17.12	16.01
							Z	1.000	1.000	1.000
							pHS	3.039	3.282	3.525

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137
15.38	15.02	13.88	13.67	13.56	13.49	14.69	14.66	14.64	13.53	13.52
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.771	4.019	4.020	4.267	4.515	4.765	4.768	5.018	5.268	5.515	5.765
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137	1.137
13.52	13.52	16.74	16.74	16.74	16.74	13.50	13.50	13.51	13.51	13.51
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.015	6.265	6.522	6.772	7.022	7.272	7.515	7.765	8.015	8.265	8.515
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 7 , 12				
1.137	1.137	1.137	1.137	1.137	1.136					
13.52	13.54	13.57	15.76	15.85	16.03					
1.000	1.000	1.000	1.000	1.000	1.000					
8.765	9.015	9.265	9.521	9.771	10.022					

225 PERIODIC ACID HIO4

-1	56.5	1.550			191.91		pHL	3.00	3.25	3.50
							RE	1.447	1.433	1.425
							t	20.93	18.81	17.55
							Z	0.976	0.986	0.992
							pHS	3.127	3.351	3.578

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.420	1.417	1.419	1.417	1.416	1.415	1.415	1.414	1.413	1.416	1.416
16.79	16.35	14.92	14.67	14.53	14.45	15.95	15.90	15.88	14.50	14.49
0.995	0.997	0.997	0.998	0.999	0.999	0.999	1.000	1.000	1.000	1.000
3.814	4.057	4.061	4.300	4.546	4.794	4.803	5.052	5.302	5.544	5.794
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.415	1.415	1.414	1.413	1.413	1.412	1.416	1.415	1.415	1.415	1.415
14.49	14.49	18.49	18.49	18.49	18.49	14.46	14.46	14.47	14.47	14.48
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.043	6.293	6.564	6.813	7.063	7.313	7.543	7.793	8.043	8.293	8.544
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 4				
1.415	1.415	1.414	1.413	1.413	1.412					
14.49	14.52	14.56	17.30	17.45	17.71					
1.000	1.000	1.000	1.000	1.000	1.000					
8.794	9.044	9.294	9.561	9.812	10.064					

226 PERMANGANIC ACID HMnO4

-1	63.4	-2.000	119.90				pHL	3.00	3.25	3.50
							RE	1.255	1.255	1.255
							t	19.92	17.86	16.67
							Z	1.000	1.000	1.000
							pHS	3.070	3.308	3.546

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.255	1.255	1.256	1.256	1.256	1.256	1.255	1.255	1.255	1.256	1.256
15.98	15.58	14.32	14.10	13.97	13.90	15.23	15.19	15.17	13.94	13.94
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.789	4.035	4.036	4.281	4.528	4.777	4.783	5.033	5.282	5.528	5.777
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.256	1.256	1.255	1.255	1.255	1.255	1.256	1.256	1.256	1.256	1.256
13.93	13.93	17.49	17.49	17.49	17.49	13.91	13.91	13.92	13.92	13.92
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.027	6.277	6.540	6.790	7.040	7.290	7.527	7.777	8.027	8.277	8.528
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.256	1.256	1.255	1.255	1.255	1.254					
13.94	13.96	13.99	16.41	16.53	16.74					
1.000	1.000	1.000	1.000	1.000	1.000					
8.778	9.028	9.278	9.538	9.789	10.040					

227 PEROXYSULFURIC ACID H2S2O8

-1	44.6	-2.000	194.13				pHL	3.00	3.25	3.50
-2	89.1	-1.000					RE	0.958	0.958	0.958
							t	35.24	31.74	29.79
							Z	2.000	2.000	2.000
							pHS	2.987	3.242	3.496

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
0.957	0.957	0.960	0.960	0.960	0.960	0.958	0.957	0.957	0.960	0.960
28.71	28.11	26.23	25.88	25.69	25.59	27.59	27.53	27.50	25.65	25.64
2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
3.748	3.999	3.999	4.250	4.501	4.751	4.750	5.000	5.250	5.501	5.751
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
0.959	0.959	0.956	0.955	0.955	0.954	0.960	0.960	0.960	0.959	0.960
25.64	25.64	31.01	31.00	31.00	31.00	25.60	25.61	25.61	25.62	25.62
2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
6.001	6.251	6.499	6.749	6.999	7.249	7.502	7.752	8.001	8.251	8.501
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
0.960	0.959	0.959	0.956	0.955	0.955					
25.64	25.67	25.71	29.34	29.48	29.73					
2.000	2.000	2.000	2.000	2.000	2.000					
8.751	9.001	9.251	9.499	9.749	9.999					

228 PERRHENIC ACID HReO4

-1	56.7	0.000	251.20				pHL	3.00	3.25	3.50
							RE	1.409	1.409	1.409
							t	21.02	18.82	17.53
							Z	0.999	1.000	1.000
							pHS	3.108	3.339	3.571

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.408	1.408	1.410	1.410	1.410	1.409	1.409	1.409	1.408	1.410	1.410
16.77	16.32	14.90	14.65	14.51	14.43	15.92	15.88	15.86	14.48	14.47
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.810	4.055	4.057	4.298	4.545	4.793	4.802	5.051	5.301	5.544	5.793
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.410	1.409	1.408	1.408	1.408	1.407	1.411	1.410	1.410	1.410	1.410
14.47	14.47	18.46	18.46	18.46	18.46	14.44	14.44	14.45	14.46	14.46
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.043	6.293	6.563	6.813	7.063	7.313	7.543	7.793	8.043	8.293	8.543
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.410	1.409	1.409	1.408	1.407	1.407					
14.47	14.50	14.54	17.27	17.42	17.68					
1.000	1.000	1.000	1.000	1.000	1.000					
8.793	9.044	9.294	9.560	9.811	10.063					

229 PHENOL C6H6O

-1	34.4	9.998	94.11				pHL	3.00	3.25	3.50
							RE	□□□□□□	□□□□□□	□□□□□□
							t	24.19	23.31	22.69
							Z	0.001	0.001	0.001
							pHS	6.781	6.867	6.945

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□
22.18	21.76	19.01	18.94	18.87	18.80	21.20	21.17	21.15	18.90	18.90
0.001	0.001	0.002	0.002	0.003	0.003	0.004	0.005	0.006	0.013	0.014
7.026	7.118	7.283	7.338	7.408	7.494	7.583	7.657	7.746	8.099	8.139

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
□□□□□□	□□□□□□	50.561	46.612	41.437	35.408	18.542	17.040	15.112	12.921	8.407
18.90	18.90	25.48	25.49	25.50	25.52	18.96	18.97	18.99	19.02	19.17
0.016	0.019	0.044	0.047	0.053	0.063	0.121	0.132	0.149	0.174	0.271
8.197	8.272	8.650	8.687	8.740	8.813	9.122	9.164	9.224	9.305	9.547

8.75	9.00	9.25	9.50	9.75	10.00
7.457	6.419	5.417	4.083	3.612	3.199
19.23	19.34	19.51	24.78	25.39	26.52
0.306	0.356	0.424	0.566	0.642	0.727
9.620	9.717	9.839	10.086	10.222	10.392

(Ref.) : 3 , 7

230 PHENOXYACETIC ACID C8H8O3

-1	27.8	3.171	152.15				pHL	3.00	3.25	3.50
							RE	4.040	3.718	3.484
							t	30.42	27.75	25.96
							Z	0.724	0.788	0.843
							pHS	3.558	3.710	3.868

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.304	3.172	3.178	3.104	3.051	3.016	3.007	2.987	2.974	2.988	2.983
24.69	23.85	20.76	20.35	20.07	19.90	23.05	22.96	22.90	20.02	20.00
0.891	0.929	0.934	0.957	0.974	0.984	0.986	0.992	0.995	0.997	0.998
4.048	4.255	4.284	4.479	4.700	4.937	4.970	5.211	5.457	5.684	5.930

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.979	2.974	2.959	2.957	2.954	2.951	2.981	2.979	2.977	2.974	2.978
19.99	19.98	28.40	28.39	28.38	28.37	19.95	19.95	19.96	19.97	20.00
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.178	6.428	6.743	6.993	7.242	7.492	7.678	7.928	8.178	8.428	8.680

8.75	9.00	9.25	9.50	9.75	10.00
2.976	2.972	2.968	2.956	2.950	2.943
20.05	20.14	20.30	26.40	27.16	28.69
1.000	1.000	1.000	1.000	1.000	1.000
8.931	9.182	9.434	9.748	10.006	10.270

(Ref.) : 11 , 1

231 PHENYLACETIC ACID C8H8O2

-1	31.7	4.405	136.15				pHL	3.00	3.25	3.50
							RE	8.332	7.058	6.099
							t	25.69	24.22	23.21
							Z	0.298	0.353	0.410
							pHS	4.011	4.119	4.222

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.270	4.539	4.126	3.774	3.437	3.151	3.086	2.907	2.777	2.704	2.660
22.44	21.87	19.02	18.83	18.66	18.54	21.25	21.19	21.15	18.64	18.63
0.476	0.555	0.616	0.675	0.744	0.814	0.831	0.883	0.925	0.957	0.973
4.337	4.472	4.580	4.691	4.834	5.010	5.061	5.248	5.462	5.715	5.927

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.630	2.610	2.589	2.583	2.578	2.574	2.595	2.593	2.591	2.588	2.592
18.62	18.61	25.95	25.94	25.93	25.93	18.58	18.58	18.59	18.60	18.62
0.984	0.991	0.995	0.997	0.999	0.999	0.999	1.000	1.000	1.000	1.000
6.160	6.403	6.713	6.957	7.205	7.455	7.649	7.898	8.148	8.398	8.650

8.75	9.00	9.25	9.50	9.75	10.00
2.590	2.587	2.584	2.576	2.572	2.567
18.66	18.73	18.85	24.07	24.61	25.65
1.000	1.000	1.000	1.000	1.000	1.000
8.900	9.151	9.403	9.706	9.962	10.222

(Ref.) : 10 , 1

232 4-PHENYLBUTYRIC ACID C10H12O2
-1 24.7 4.757 164.20

pHL	3.00	3.25	3.50
RE	14.144	11.861	10.133
t	30.42	28.50	27.20
Z	0.225	0.270	0.317
pHS	4.203	4.305	4.402

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
8.629	7.289	6.458	5.816	5.184	4.624	4.457	4.098	3.822	3.641	3.544
26.22	25.50	21.82	21.60	21.41	21.27	24.78	24.71	24.67	21.43	21.42
0.373	0.444	0.507	0.565	0.636	0.717	0.743	0.811	0.872	0.925	0.951
4.510	4.636	4.743	4.843	4.971	5.129	5.189	5.358	5.556	5.811	6.005

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.474	3.428	3.377	3.364	3.354	3.346	3.384	3.380	3.376	3.372	3.378
21.41	21.40	30.93	30.92	30.91	30.90	21.37	21.37	21.38	21.40	21.44
0.970	0.982	0.992	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.229	6.467	6.791	7.033	7.280	7.529	7.708	7.957	8.207	8.457	8.710

8.75	9.00	9.25	9.50	9.75	10.00
3.374	3.370	3.364	3.346	3.339	3.328
21.50	21.62	21.83	28.87	29.94	32.19
1.000	1.000	1.000	1.000	1.000	1.000
8.961	9.212	9.465	9.790	10.050	10.320

(Ref.) : 11 , 7

233 2-PHENYLPROPIONIC ACID C9H10O2
-1 26.5 2.237 150.20

pHL	3.00	3.25	3.50
RE	3.294	3.230	3.187
t	32.83	29.33	27.08
Z	0.942	0.962	0.975
pHS	3.417	3.604	3.797

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.158	3.138	3.159	3.147	3.138	3.132	3.125	3.120	3.115	3.137	3.134
25.57	24.63	21.44	20.95	20.63	20.45	23.77	23.67	23.60	20.58	20.56
0.985	0.991	0.991	0.995	0.997	0.998	0.998	0.999	0.999	1.000	1.000
4.007	4.235	4.244	4.462	4.697	4.940	4.973	5.219	5.467	5.692	5.940

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.132	3.128	3.111	3.109	3.107	3.103	3.136	3.135	3.132	3.129	3.134
20.54	20.54	29.39	29.38	29.37	29.36	20.50	20.50	20.51	20.53	20.56
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.189	6.439	6.757	7.007	7.256	7.506	7.689	7.939	8.189	8.439	8.692

8.75	9.00	9.25	9.50	9.75	10.00
3.131	3.127	3.123	3.108	3.102	3.093
20.62	20.72	20.90	27.35	28.22	30.01
1.000	1.000	1.000	1.000	1.000	1.000
8.943	9.194	9.446	9.765	10.023	10.290

(Ref.) : 11 , 3

234 3-PHENYLPROPIONIC ACID C9H10O2
-1 26.5 4.664 150.20

pHL	3.00	3.25	3.50
RE	12.233	10.283	8.810
t	28.94	27.17	25.96
Z	0.243	0.290	0.339
pHS	4.151	4.255	4.353

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.528	6.390	5.693	5.148	4.614	4.144	4.013	3.714	3.488	3.344	3.265
25.05	24.38	20.95	20.74	20.56	20.42	23.69	23.62	23.58	20.57	20.55
0.399	0.472	0.536	0.594	0.665	0.744	0.768	0.832	0.888	0.935	0.958
4.462	4.590	4.698	4.801	4.932	5.094	5.152	5.326	5.528	5.783	5.982

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.209	3.173	3.133	3.121	3.113	3.107	3.139	3.136	3.133	3.129	3.134
20.54	20.54	29.38	29.38	29.37	29.36	20.50	20.50	20.51	20.53	20.56
0.974	0.985	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.208	6.448	6.768	7.011	7.258	7.507	7.691	7.940	8.189	8.439	8.692

8.75	9.00	9.25	9.50	9.75	10.00
3.131	3.127	3.123	3.108	3.102	3.093
20.62	20.72	20.90	27.35	28.22	30.01
1.000	1.000	1.000	1.000	1.000	1.000
8.943	9.194	9.446	9.765	10.023	10.290

(Ref.) : 11 , 1

235 PHOSPHORIC ACID (S) H3PO4 98.00

-1	35.1	2.120					pHL	3.00	3.25	3.50
-2	61.5	7.470					RE	2.449	2.401	2.369
-3	71.5	12.360					t	27.20	24.38	22.60
							Z	0.944	0.964	0.977
							pHS	3.313	3.510	3.711

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.348	2.333	2.344	2.336	2.328	2.322	2.319	2.312	2.302	2.300	2.278
21.45	20.74	18.38	18.01	17.79	17.68	20.16	20.13	20.18	18.06	18.31
0.986	0.992	0.993	0.996	0.999	1.002	1.002	1.005	1.010	1.019	1.034
3.929	4.162	4.170	4.394	4.633	4.878	4.903	5.150	5.398	5.645	5.893
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.241	2.183	2.037	1.936	1.825	1.715	1.619	1.559	1.510	1.475	1.456
18.74	19.42	28.10	29.47	30.97	32.47	26.37	27.12	27.72	28.15	28.43
1.058	1.099	1.209	1.300	1.411	1.536	1.686	1.775	1.852	1.909	1.947
6.141	6.389	6.770	6.975	7.183	7.397	7.665	7.860	8.080	8.314	8.564
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 4				
1.443	1.434	1.429	1.419	1.415	1.412					
28.62	28.76	28.90	34.40	34.74	35.32					
1.969	1.983	1.991	1.997	2.002	2.007					
8.806	9.053	9.302	9.568	9.818	10.070					

236 PHOSPHOROUS ACID H3PO3 82.00

-1	40.0	2.000					pHL	3.00	3.25	3.50
-2	65.4	7.000					RE	2.120	2.083	2.059
							t	25.15	22.56	20.95
							Z	0.952	0.970	0.982
							pHS	3.262	3.465	3.673

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.043	2.032	2.040	2.032	2.026	2.018	2.016	2.006	1.990	1.972	1.933
19.94	19.33	17.26	16.95	16.79	16.74	18.91	18.99	19.19	17.61	18.23
0.990	0.995	0.995	0.999	1.003	1.008	1.009	1.016	1.030	1.054	1.093
3.895	4.130	4.138	4.366	4.607	4.853	4.874	5.122	5.371	5.638	5.884
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.875	1.796	1.648	1.573	1.501	1.440	1.407	1.380	1.361	1.349	1.344
19.17	20.44	29.42	30.83	32.18	33.32	26.94	27.39	27.70	27.90	28.02
1.152	1.240	1.423	1.532	1.648	1.756	1.848	1.903	1.941	1.966	1.980
6.127	6.368	6.730	6.918	7.123	7.344	7.596	7.815	8.051	8.295	8.546
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 6				
1.339	1.336	1.334	1.327	1.324	1.322					
28.11	28.19	28.28	33.38	33.63	34.08					
1.989	1.994	1.996	1.998	1.999	1.999					
8.793	9.042	9.292	9.555	9.805	10.056					

237 PHTHALIC ACID C8H6O4 166.13

-1	28.1	2.950					pHL	3.00	3.25	3.50
-2	52.9	5.408					RE	3.608	3.360	3.173
							t	30.89	28.17	26.48
							Z	0.807	0.869	0.924
							pHS	3.499	3.661	3.831

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.013	2.866	2.857	2.722	2.565	2.390	2.353	2.186	2.033	1.903	1.829
25.50	25.19	22.20	22.54	23.34	24.50	28.03	29.31	30.55	28.70	29.29
0.977	1.034	1.047	1.108	1.190	1.297	1.318	1.441	1.572	1.721	1.805
4.022	4.236	4.278	4.481	4.700	4.925	4.969	5.183	5.403	5.681	5.879
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.772	1.733	1.695	1.681	1.671	1.664	1.686	1.683	1.681	1.679	1.682
29.75	30.07	39.66	39.76	39.81	39.82	30.47	30.49	30.50	30.51	30.54
1.874	1.923	1.958	1.975	1.986	1.992	1.995	1.997	1.998	1.999	2.000
6.101	6.337	6.625	6.862	7.106	7.354	7.576	7.825	8.074	8.324	8.575
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.680	1.678	1.675	1.665	1.661	1.658					
30.57	30.62	30.73	37.18	37.56	38.27					
2.000	2.000	2.000	2.000	2.000	2.000					
8.825	9.075	9.325	9.600	9.852	10.105					

238 PICRIC ACID C6H3N3O7

-1	31.5	0.708	229.11				pHL	3.00	3.25	3.50
							RE	2.601	2.598	2.597
							t	29.50	26.24	24.20
							Z	0.998	0.999	0.999
							pHS	3.317	3.522	3.729

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.596	2.594	2.609	2.608	2.606	2.604	2.601	2.598	2.596	2.611	2.609
22.90	22.09	19.45	19.02	18.76	18.60	21.37	21.29	21.24	18.71	18.69
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.950	4.184	4.189	4.415	4.654	4.900	4.927	5.174	5.423	5.651	5.900
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.607	2.605	2.595	2.593	2.592	2.589	2.611	2.610	2.608	2.605	2.609
18.68	18.68	26.06	26.05	26.05	26.04	18.64	18.64	18.65	18.66	18.68
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.149	6.399	6.707	6.956	7.206	7.456	7.649	7.899	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
2.607	2.605	2.602	2.593	2.589	2.584					
18.72	18.79	18.92	24.17	24.72	25.78					
1.000	1.000	1.000	1.000	1.000	1.000					
8.902	9.153	9.404	9.708	9.964	10.224					

239 PIMELIC ACID C7H12O4

-1	24.0	4.509	160.17				pHL	3.00	3.25	3.50
-2	49.9	5.312					RE	10.544	8.738	7.364
							t	32.34	30.57	29.52
							Z	0.313	0.379	0.452
							pHS	4.080	4.184	4.283

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.166	5.095	4.412	3.882	3.359	2.892	2.764	2.458	2.215	2.031	1.947
28.90	28.72	25.48	25.80	26.34	27.10	31.04	31.83	32.63	30.12	30.50
0.542	0.660	0.773	0.882	1.026	1.199	1.254	1.418	1.580	1.750	1.830
4.392	4.519	4.629	4.731	4.861	5.020	5.074	5.239	5.433	5.704	5.892
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.884	1.842	1.802	1.788	1.779	1.772	1.797	1.794	1.792	1.789	1.793
30.80	31.00	41.15	41.20	41.22	41.21	31.25	31.26	31.26	31.27	31.30
1.894	1.937	1.967	1.981	1.989	1.994	1.996	1.998	1.999	1.999	2.000
6.111	6.347	6.637	6.875	7.120	7.368	7.586	7.835	8.084	8.334	8.585
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.791	1.788	1.785	1.773	1.769	1.765					
31.34	31.40	31.51	38.41	38.85	39.66					
2.000	2.000	2.000	2.000	2.000	2.000					
8.835	9.085	9.336	9.614	9.866	10.120					

240 PROPIONIC ACID (S) C3H6O2

-1	37.1	4.874	74.08				pHL	3.00	3.25	3.50
							RE	11.190	9.352	7.973
							t	22.76	21.71	20.98
							Z	0.187	0.224	0.264
							pHS	4.218	4.316	4.407

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.766	5.675	4.747	4.278	3.796	3.344	3.185	2.895	2.653	2.439	2.359
20.41	19.97	17.50	17.38	17.27	17.17	19.45	19.41	19.37	17.24	17.23
0.312	0.373	0.450	0.501	0.566	0.645	0.678	0.748	0.818	0.897	0.928
4.507	4.624	4.760	4.846	4.959	5.100	5.164	5.312	5.491	5.775	5.945
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.296	2.253	2.217	2.203	2.195	2.189	2.201	2.198	2.196	2.194	2.196
17.22	17.22	23.43	23.43	23.43	23.42	17.18	17.19	17.19	17.20	17.22
0.954	0.972	0.986	0.992	0.995	0.997	0.998	0.999	0.999	1.000	1.000
6.153	6.383	6.688	6.922	7.166	7.413	7.618	7.866	8.116	8.366	8.617
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 1				
2.195	2.193	2.191	2.186	2.184	2.180					
17.24	17.30	17.39	21.74	22.11	22.79					
1.000	1.000	1.000	1.000	1.000	1.000					
8.867	9.118	9.369	9.661	9.914	10.171					

241 3-PROPYLGLUTARIC ACID C8H1404 174.20

-1	23.5	4.312					pHL	3.00	3.25	3.50
-2	47.0	5.386					RE	9.319	7.837	6.702
							t	32.96	30.96	29.74
							Z	0.365	0.437	0.513
							pHS	4.000	4.109	4.215

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.710	4.824	4.360	3.883	3.416	2.998	2.890	2.599	2.363	2.181	2.089
29.00	28.75	25.31	25.63	26.23	27.11	31.24	32.21	33.18	30.66	31.13
0.606	0.724	0.812	0.918	1.053	1.212	1.257	1.410	1.564	1.729	1.813
4.333	4.472	4.571	4.688	4.835	5.009	5.062	5.241	5.442	5.713	5.904
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.019	1.972	1.926	1.910	1.899	1.891	1.920	1.917	1.914	1.911	1.915
31.50	31.75	42.61	42.68	42.70	42.70	32.08	32.09	32.10	32.11	32.15
1.881	1.928	1.962	1.978	1.987	1.993	1.996	1.998	1.999	1.999	2.000
6.123	6.359	6.652	6.890	7.135	7.383	7.597	7.846	8.095	8.345	8.596
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 7				
1.912	1.909	1.906	1.892	1.887	1.882					
32.18	32.25	32.38	39.77	40.27	41.20					
2.000	2.000	2.000	2.000	2.000	2.000					
8.846	9.096	9.347	9.629	9.882	10.136					

242 PROPYLMALONIC ACID C6H1004 146.14

-1	26.0	2.971					pHL	3.00	3.25	3.50
-2	52.0	5.845					RE	3.937	3.683	3.496
							t	32.46	29.45	27.50
							Z	0.799	0.857	0.905
							pHS	3.525	3.687	3.855

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.345	3.219	3.225	3.120	2.998	2.846	2.809	2.627	2.427	2.188	2.060
26.22	25.52	22.25	22.15	22.43	23.12	26.72	27.78	29.03	27.59	28.42
0.947	0.986	0.992	1.028	1.072	1.134	1.148	1.234	1.345	1.522	1.627
4.045	4.258	4.290	4.494	4.719	4.952	4.998	5.223	5.448	5.753	5.934
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.947	1.859	1.776	1.743	1.721	1.706	1.724	1.719	1.715	1.711	1.714
29.16	29.74	39.75	39.96	40.08	40.15	30.65	30.68	30.70	30.72	30.75
1.731	1.820	1.901	1.938	1.963	1.979	1.987	1.993	1.996	1.998	1.999
6.138	6.361	6.660	6.880	7.117	7.361	7.583	7.829	8.078	8.327	8.578
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 12 , 2				
1.712	1.709	1.707	1.696	1.692	1.689					
30.79	30.84	30.95	37.54	37.93	38.67					
1.999	2.000	2.000	2.000	2.000	2.000					
8.828	9.078	9.328	9.604	9.856	10.109					

243 PROPYLSULFONIC ACID C3H803S 124.15

-1	38.5	-2.000					pHL	3.00	3.25	3.50
							RE	2.104	2.104	2.104
							t	26.01	23.17	21.44
							Z	1.000	1.000	1.000
							pHS	3.241	3.455	3.670

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.104	2.103	2.111	2.111	2.110	2.109	2.107	2.106	2.104	2.113	2.112
20.35	19.69	17.55	17.20	16.99	16.87	19.11	19.04	19.00	16.94	16.93
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.897	4.135	4.139	4.370	4.612	4.858	4.879	5.127	5.376	5.610	5.859
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.111	2.110	2.104	2.103	2.102	2.101	2.113	2.112	2.111	2.110	2.112
16.93	16.92	22.90	22.90	22.90	22.89	16.89	16.89	16.90	16.91	16.92
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.108	6.358	6.653	6.902	7.152	7.402	7.608	7.858	8.108	8.358	8.609
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
2.111	2.109	2.108	2.103	2.101	2.098					
16.95	16.99	17.08	21.26	21.59	22.22					
1.000	1.000	1.000	1.000	1.000	1.000					
8.860	9.110	9.361	9.651	9.904	10.160					

244 PYRAZOLE-2,3-DICARBOXYLIC ACID C5H5N2O4 157.11

-1	33.8	1.000					pHL	3.00	3.25	3.50
-2	56.0	4.228					RE	2.258	2.180	2.086
							t	30.82	28.74	28.14
							Z	1.126	1.194	1.283
							pHS	3.286	3.495	3.702

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.980	1.871	1.866	1.782	1.712	1.660	1.652	1.618	1.596	1.597	1.589
28.43	29.23	26.53	27.30	28.00	28.56	31.83	32.22	32.46	29.65	29.73
1.396	1.525	1.549	1.663	1.767	1.850	1.855	1.911	1.947	1.969	1.982
3.916	4.137	4.176	4.380	4.600	4.833	4.853	5.088	5.331	5.576	5.819
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.584	1.580	1.568	1.566	1.563	1.560	1.581	1.580	1.579	1.577	1.580
29.78	29.81	38.66	38.65	38.64	38.62	29.81	29.81	29.81	29.82	29.84
1.990	1.994	1.997	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000
6.066	6.315	6.591	6.840	7.090	7.339	7.564	7.814	8.064	8.314	8.565
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10				
1.578	1.577	1.575	1.565	1.563	1.560					
29.87	29.92	30.02	36.07	36.40	37.03					
2.000	2.000	2.000	2.000	2.000	2.000					
8.815	9.065	9.315	9.587	9.838	10.091					

245 PYROPHOSPHORIC ACID H4P2O7 177.98

-1	24.9	1.520					pHL	3.00	3.25	3.50
-2	57.9	2.360					RE	1.604	1.568	1.546
-3	75.3	6.750					t	42.47	38.28	35.77
-4	88.8	9.290					Z	1.895	1.935	1.962
							pHS	3.163	3.379	3.601

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.531	1.521	1.533	1.527	1.522	1.516	1.511	1.504	1.493	1.492	1.471
34.26	33.38	30.38	29.92	29.70	29.66	32.88	33.02	33.36	31.06	32.00
1.979	1.990	1.991	1.999	2.007	2.018	2.018	2.035	2.062	2.108	2.178
3.834	4.075	4.080	4.317	4.562	4.810	4.822	5.070	5.319	5.576	5.822
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.441	1.405	1.350	1.319	1.292	1.272	1.286	1.275	1.265	1.253	1.245
33.32	34.94	46.74	48.38	49.73	50.78	41.24	41.98	42.87	44.05	45.65
2.279	2.408	2.579	2.705	2.814	2.901	2.971	3.034	3.106	3.198	3.321
6.067	6.312	6.605	6.831	7.066	7.308	7.552	7.796	8.043	8.292	8.547
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 4				
1.230	1.215	1.201	1.174	1.164	1.157					
47.45	49.26	50.91	60.49	61.66	62.82					
3.463	3.609	3.737	3.835	3.900	3.942					
8.793	9.040	9.288	9.544	9.792	10.041					

246 PYRUVIC ACID C3H4O3 88.06

-1	42.3	2.490					pHL	3.00	3.25	3.50
							RE	2.171	2.078	2.016
							t	23.90	21.67	20.25
							Z	0.876	0.916	0.945
							pHS	3.301	3.489	3.683

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.973	1.946	1.951	1.935	1.925	1.918	1.917	1.913	1.910	1.916	1.914
19.31	18.73	16.78	16.47	16.28	16.18	18.20	18.14	18.11	16.24	16.23
0.965	0.979	0.980	0.988	0.993	0.996	0.996	0.998	0.999	0.999	1.000
3.896	4.125	4.139	4.361	4.599	4.843	4.862	5.108	5.357	5.593	5.841
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.913	1.912	1.908	1.907	1.906	1.905	1.915	1.914	1.913	1.912	1.914
16.23	16.23	21.65	21.64	21.64	21.64	16.19	16.20	16.20	16.21	16.22
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.091	6.341	6.629	6.879	7.129	7.379	7.591	7.841	8.091	8.341	8.592
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 7				
1.913	1.912	1.910	1.907	1.906	1.903					
16.24	16.28	16.35	20.12	20.38	20.88					
1.000	1.000	1.000	1.000	1.000	1.000					
8.842	9.092	9.343	9.627	9.879	10.134					

247 SACCHARIN C7H5NO3S

-1	31.3	2.432	183.20				pHL	3.00	3.25	3.50
							RE	2.874	2.783	2.722
							t	29.06	26.12	24.23
							Z	0.906	0.937	0.958
							pHS	3.381	3.566	3.757

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.679	2.651	2.665	2.648	2.637	2.629	2.625	2.620	2.615	2.630	2.628
22.96	22.17	19.49	19.08	18.82	18.67	21.45	21.37	21.32	18.77	18.75
0.974	0.984	0.985	0.991	0.995	0.997	0.997	0.998	0.999	0.999	1.000
3.966	4.194	4.205	4.424	4.659	4.903	4.931	5.176	5.425	5.654	5.902
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.625	2.623	2.612	2.611	2.609	2.607	2.629	2.627	2.626	2.623	2.627
18.74	18.74	26.17	26.16	26.16	26.15	18.70	18.71	18.71	18.73	18.75
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.151	6.401	6.709	6.958	7.208	7.458	7.651	7.901	8.151	8.401	8.653
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.625	2.622	2.619	2.610	2.607	2.601					
18.79	18.86	18.98	24.28	24.83	25.91					
1.000	1.000	1.000	1.000	1.000	1.000					
8.903	9.154	9.406	9.710	9.966	10.226					

248 SALICYLIC ACID C7H6O3

-1	35.4	3.107	138.12				pHL	3.00	3.25	3.50
							RE	3.155	2.895	2.708
							t	25.79	23.67	22.26
							Z	0.721	0.787	0.843
							pHS	3.485	3.641	3.802

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.565	2.461	2.460	2.403	2.363	2.336	2.332	2.317	2.307	2.314	2.310
21.27	20.61	18.22	17.89	17.68	17.55	19.99	19.92	19.88	17.63	17.62
0.891	0.930	0.935	0.958	0.974	0.985	0.986	0.992	0.995	0.997	0.998
3.985	4.193	4.226	4.423	4.646	4.884	4.910	5.151	5.397	5.631	5.877
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.308	2.305	2.297	2.296	2.294	2.292	2.308	2.307	2.306	2.304	2.307
17.61	17.61	24.14	24.14	24.13	24.13	17.57	17.58	17.58	17.59	17.61
0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.125	6.375	6.675	6.925	7.174	7.424	7.625	7.875	8.125	8.375	8.626
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
2.305	2.304	2.301	2.296	2.293	2.289					
17.64	17.70	17.79	22.39	22.80	23.57					
1.000	1.000	1.000	1.000	1.000	1.000					
8.877	9.127	9.379	9.674	9.928	10.186					

249 SEBACIC ACID C10H18O4

-1	20.7	4.530	202.25				pHL	3.00	3.25	3.50
-2	44.9	5.380					RE	12.173	10.107	8.526
							t	36.02	33.79	32.42
							Z	0.315	0.380	0.452
							pHS	4.111	4.214	4.314

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.143	5.907	5.173	4.540	3.919	3.364	3.206	2.839	2.545	2.318	2.212
31.57	31.21	27.33	27.58	28.05	28.74	33.18	33.91	34.65	31.68	32.04
0.541	0.657	0.759	0.867	1.008	1.177	1.232	1.394	1.556	1.731	1.815
4.425	4.553	4.655	4.760	4.892	5.051	5.107	5.272	5.464	5.733	5.918
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.132	2.079	2.026	2.008	1.996	1.987	2.020	2.016	2.013	2.009	2.014
32.33	32.52	43.90	43.94	43.95	43.93	32.77	32.78	32.79	32.79	32.83
1.883	1.930	1.963	1.978	1.988	1.993	1.996	1.998	1.999	1.999	2.000
6.135	6.368	6.665	6.902	7.147	7.395	7.606	7.854	8.104	8.354	8.605
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 12				
2.011	2.008	2.004	1.988	1.983	1.978					
32.87	32.95	33.09	40.88	41.43	42.48					
2.000	2.000	2.000	2.000	2.000	2.000					
8.855	9.105	9.356	9.642	9.894	10.149					

250 SELENIC ACID H2SeO4 144.97

-1	41.0	0.000					pHL	3.00	3.25	3.50
-2	80.5	2.050					RE	1.100	1.085	1.077
							t	36.21	32.80	30.84
							Z	1.933	1.961	1.977
							pHS	3.038	3.278	3.521

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.072	1.068	1.073	1.071	1.070	1.069	1.067	1.066	1.065	1.069	1.069
29.72	29.09	26.99	26.63	26.42	26.31	28.54	28.48	28.45	26.39	26.38
1.987	1.993	1.993	1.996	1.998	1.999	1.999	1.999	2.000	2.000	2.000
3.768	4.016	4.017	4.265	4.514	4.763	4.765	5.015	5.264	5.513	5.763
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.069	1.068	1.063	1.063	1.062	1.061	1.069	1.069	1.069	1.068	1.069
26.38	26.38	32.36	32.35	32.35	32.34	26.34	26.34	26.35	26.36	26.36
2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
6.013	6.263	6.516	6.766	7.016	7.266	7.513	7.763	8.013	8.263	8.513
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 4				
1.069	1.068	1.068	1.064	1.063	1.062					
26.38	26.41	26.46	30.51	30.68	30.97					
2.000	2.000	2.000	2.000	2.000	2.000					
8.763	9.013	9.263	9.516	9.766	10.016					

251 SELENIOUS ACID H2SeO3 128.97

-1	41.2	2.620					pHL	3.00	3.25	3.50
-2	60.5	8.450					RE	2.301	2.184	2.105
							t	24.12	21.93	20.52
							Z	0.848	0.895	0.929
							pHS	3.331	3.512	3.701

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.049	2.012	2.018	1.997	1.983	1.974	1.973	1.967	1.963	1.968	1.966
19.58	18.99	16.98	16.67	16.48	16.37	18.45	18.40	18.37	16.47	16.48
0.955	0.973	0.974	0.984	0.991	0.995	0.995	0.998	0.999	1.001	1.003
3.908	4.135	4.152	4.370	4.605	4.849	4.869	5.114	5.363	5.599	5.848
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.963	1.958	1.946	1.935	1.915	1.885	1.847	1.790	1.723	1.653	1.587
16.52	16.59	22.41	22.72	23.24	24.07	19.31	20.67	22.28	23.96	25.64
1.006	1.010	1.020	1.035	1.061	1.104	1.180	1.272	1.390	1.523	1.667
6.097	6.347	6.648	6.897	7.145	7.393	7.660	7.889	8.117	8.348	8.607
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11				
1.541	1.506	1.482	1.460	1.449	1.442					
26.78	27.66	28.30	34.15	34.66	35.32					
1.772	1.854	1.912	1.950	1.971	1.984					
8.832	9.068	9.311	9.577	9.824	10.075					

252 SELENOCYANIC ACID HSeCN 105.99

-1	67.1	0.000					pHL	3.00	3.25	3.50
							RE	1.185	1.184	1.184
							t	19.40	17.41	16.27
							Z	0.999	1.000	1.000
							pHS	3.052	3.293	3.534

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.184	1.184	1.185	1.184	1.184	1.184	1.184	1.184	1.184	1.185	1.185
15.62	15.24	14.05	13.84	13.72	13.66	14.91	14.87	14.85	13.69	13.69
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.778	4.026	4.027	4.272	4.521	4.770	4.774	5.024	5.274	5.520	5.770
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.184	1.184	1.184	1.184	1.184	1.184	1.185	1.185	1.184	1.184	1.185
13.69	13.69	17.04	17.04	17.04	17.04	13.66	13.66	13.67	13.67	13.67
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.020	6.270	6.529	6.779	7.029	7.279	7.520	7.770	8.020	8.270	8.520
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 12				
1.184	1.184	1.184	1.184	1.184	1.183					
13.69	13.71	13.74	16.02	16.12	16.31					
1.000	1.000	1.000	1.000	1.000	1.000					
8.770	9.020	9.270	9.528	9.778	10.029					

253 SORBIC ACID C6H8O2 112.13

-1	33.4	4.770					pHL	3.00	3.25	3.50
							RE	11.103	9.298	7.942
							t	24.46	23.21	22.35
							Z	0.210	0.252	0.296
							pHS	4.177	4.277	4.372

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.758	5.696	4.888	4.413	3.933	3.494	3.356	3.074	2.847	2.671	2.595
21.68	21.18	18.45	18.30	18.16	18.06	20.61	20.56	20.52	18.15	18.14
0.349	0.415	0.489	0.543	0.611	0.690	0.719	0.787	0.852	0.915	0.943
4.475	4.596	4.722	4.815	4.935	5.085	5.146	5.304	5.493	5.766	5.949
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.538	2.499	2.465	2.454	2.446	2.440	2.457	2.455	2.453	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.964	0.979	0.990	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000
6.165	6.400	6.709	6.947	7.193	7.441	7.639	7.888	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

254 SUBERIC ACID C8H14O4 174.20

-1	22.5	4.517					pHL	3.00	3.25	3.50
-2	47.2	5.403					RE	11.348	9.435	7.974
							t	33.79	31.79	30.58
							Z	0.311	0.375	0.446
							pHS	4.095	4.199	4.299

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.697	5.554	4.857	4.276	3.703	3.188	3.042	2.698	2.420	2.199	2.099
29.83	29.55	26.00	26.27	26.78	27.54	31.72	32.54	33.37	30.75	31.16
0.533	0.646	0.749	0.854	0.991	1.158	1.213	1.373	1.537	1.718	1.804
4.409	4.538	4.643	4.748	4.880	5.041	5.096	5.262	5.454	5.726	5.910
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.022	1.970	1.920	1.903	1.891	1.883	1.911	1.908	1.905	1.902	1.906
31.50	31.72	42.52	42.58	42.60	42.60	32.02	32.03	32.04	32.05	32.08
1.875	1.925	1.960	1.977	1.987	1.992	1.995	1.997	1.999	1.999	2.000
6.126	6.359	6.654	6.890	7.134	7.382	7.596	7.845	8.094	8.344	8.595
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 7				
1.903	1.900	1.897	1.883	1.879	1.874					
32.12	32.19	32.32	39.67	40.16	41.09					
2.000	2.000	2.000	2.000	2.000	2.000					
8.845	9.096	9.346	9.628	9.880	10.135					

255 SUCCINIC ACID (S) C4H6O4 118.09

-1	33.0	4.207					pHL	3.00	3.25	3.50
-2	60.9	5.638					RE	6.629	5.619	4.856
							t	25.62	24.26	23.41
							Z	0.363	0.430	0.500
							pHS	3.914	4.025	4.133

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.193	3.604	3.280	2.972	2.667	2.385	2.316	2.104	1.916	1.728	1.643
22.86	22.62	20.16	20.38	20.86	21.69	24.71	25.82	27.11	26.16	26.93
0.583	0.683	0.761	0.846	0.954	1.082	1.118	1.251	1.399	1.600	1.702
4.254	4.397	4.504	4.625	4.779	4.962	5.015	5.201	5.407	5.704	5.885
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.571	1.520	1.474	1.455	1.443	1.435	1.448	1.445	1.443	1.441	1.443
27.60	28.09	36.49	36.67	36.78	36.84	28.82	28.84	28.86	28.88	28.89
1.797	1.871	1.929	1.957	1.975	1.986	1.992	1.995	1.997	1.998	1.999
6.095	6.323	6.608	6.837	7.078	7.324	7.555	7.803	8.052	8.301	8.552
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
1.441	1.440	1.439	1.431	1.429	1.426					
28.92	28.97	29.05	34.56	34.84	35.36					
2.000	2.000	2.000	2.000	2.000	2.000					
8.802	9.052	9.302	9.569	9.820	10.071					

256 SULFAMIC ACID (S) HSO3NH2

-1 50.3 -2.000 97.09

pHL	3.00	3.25	3.50
RE	1.594	1.594	1.594
t	22.36	19.98	18.57
Z	1.000	1.000	1.000
pHS	3.147	3.373	3.600

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.594	1.593	1.597	1.597	1.596	1.596	1.595	1.595	1.594	1.598	1.597
17.72	17.22	15.61	15.33	15.17	15.08	16.77	16.72	16.69	15.13	15.12
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.835	4.078	4.080	4.318	4.563	4.811	4.824	5.073	5.322	5.562	5.812
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.597	1.596	1.594	1.594	1.593	1.592	1.598	1.597	1.597	1.596	1.597
15.12	15.12	19.64	19.64	19.64	19.64	15.09	15.09	15.10	15.11	15.11
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.061	6.311	6.589	6.838	7.088	7.338	7.561	7.811	8.061	8.311	8.562
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 12				
1.597	1.596	1.595	1.594	1.593	1.591					
15.13	15.16	15.21	18.32	18.50	18.84					
1.000	1.000	1.000	1.000	1.000	1.000					
8.812	9.062	9.313	9.586	9.837	10.090					

257 SULFANILIC ACID C6H7NO3S

-1 33.7 3.227 173.19

pHL	3.00	3.25	3.50
RE	3.489	3.175	2.946
t	26.44	24.32	22.89
Z	0.685	0.754	0.814
pHS	3.532	3.681	3.835

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.768	2.636	2.630	2.558	2.505	2.471	2.465	2.445	2.432	2.439	2.434
21.88	21.20	18.67	18.34	18.11	17.98	20.55	20.47	20.43	18.07	18.05
0.868	0.913	0.920	0.947	0.967	0.981	0.982	0.990	0.994	0.996	0.998
4.011	4.214	4.252	4.443	4.661	4.896	4.925	5.164	5.410	5.642	5.888
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.431	2.428	2.419	2.417	2.415	2.413	2.431	2.430	2.429	2.427	2.430
18.05	18.04	24.92	24.91	24.91	24.90	18.01	18.01	18.02	18.03	18.05
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.136	6.385	6.688	6.938	7.188	7.437	7.635	7.885	8.135	8.385	8.637
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
2.428	2.426	2.423	2.417	2.413	2.409					
18.08	18.14	18.25	23.11	23.57	24.45					
1.000	1.000	1.000	1.000	1.000	1.000					
8.887	9.138	9.389	9.688	9.943	10.201					

258 m-SULFANILIC ACID C6H7NO3S

-1 33.4 3.740 173.19

pHL	3.00	3.25	3.50
RE	4.748	4.158	3.717
t	25.68	23.95	22.77
Z	0.503	0.576	0.646
pHS	3.717	3.844	3.971

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.350	3.049	2.973	2.815	2.684	2.589	2.576	2.521	2.486	2.480	2.468
21.90	21.28	18.65	18.39	18.19	18.06	20.65	20.57	20.53	18.15	18.14
0.719	0.792	0.818	0.866	0.909	0.943	0.947	0.968	0.981	0.989	0.994
4.116	4.288	4.358	4.513	4.703	4.920	4.955	5.180	5.419	5.656	5.894
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.460	2.454	2.443	2.441	2.439	2.436	2.454	2.453	2.452	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.140	6.388	6.692	6.941	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

259 o-SULFANILIC ACID C6H7NO3S

-1	33.4	7.488								

pHL	3.00	3.25	3.50							
RE	□□□□□□	□□□□□□	□□□□□□							
t	23.80	22.79	22.08							
Z	0.011	0.013	0.016							
pHS	5.518	5.605	5.684							

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	96.602	67.988	59.744	50.784	41.726	34.677	29.299	23.954	12.186	11.128
21.52	21.08	18.34	18.25	18.17	18.09	20.52	20.49	20.47	18.18	18.18
0.019	0.023	0.033	0.038	0.045	0.055	0.066	0.078	0.096	0.191	0.210
5.767	5.861	6.019	6.077	6.151	6.240	6.326	6.405	6.501	6.844	6.893
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
9.820	8.393	4.981	4.626	4.196	3.748	3.156	2.989	2.822	2.685	2.586
18.17	18.17	24.93	24.94	24.95	24.97	18.11	18.11	18.11	18.12	18.14
0.238	0.280	0.477	0.515	0.569	0.639	0.769	0.814	0.863	0.909	0.946
6.963	7.055	7.422	7.487	7.580	7.706	7.976	8.092	8.252	8.448	8.696
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.531	2.495	2.473	2.453	2.443	2.436					
18.17	18.23	18.34	23.26	23.72	24.63					
0.967	0.981	0.989	0.994	0.997	0.998					
8.915	9.152	9.397	9.695	9.947	10.205					

260 SULFURIC ACID H2SO4

-1	52.0	-3.000								
-2	82.9	1.921								

pHL	3.00	3.25	3.50							
RE	1.052	1.044	1.039							
t	35.73	32.38	30.47							
Z	1.948	1.970	1.983							
pHS	3.020	3.266	3.513							

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.036	1.034	1.038	1.037	1.036	1.036	1.034	1.033	1.032	1.036	1.036
29.39	28.78	26.74	26.39	26.20	26.09	28.25	28.20	28.16	26.17	26.16
1.990	1.994	1.994	1.997	1.998	1.999	1.999	1.999	2.000	2.000	2.000
3.761	4.011	4.011	4.260	4.510	4.760	4.760	5.010	5.260	5.510	5.760
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.036	1.035	1.031	1.031	1.030	1.029	1.036	1.036	1.036	1.036	1.036
26.16	26.16	31.95	31.94	31.94	31.93	26.11	26.12	26.13	26.13	26.14
2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
6.010	6.260	6.511	6.761	7.011	7.261	7.510	7.760	8.010	8.260	8.510
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 1 , 4				
1.036	1.035	1.035	1.031	1.030	1.030					
26.15	26.19	26.24	30.16	30.31	30.59					
2.000	2.000	2.000	2.000	2.000	1.999					
8.760	9.010	9.260	9.511	9.761	10.011					

261 SULFUROUS ACID H2SO3

-1	51.8	1.780								
-2	74.6	6.991								

pHL	3.00	3.25	3.50							
RE	1.603	1.580	1.566							
t	21.82	19.62	18.29							
Z	0.964	0.978	0.987							
pHS	3.165	3.382	3.603							

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.557	1.551	1.555	1.551	1.548	1.544	1.544	1.539	1.531	1.523	1.505
17.49	17.01	15.45	15.20	15.08	15.05	16.71	16.78	16.96	15.77	16.32
0.993	0.997	0.997	1.000	1.003	1.008	1.008	1.015	1.028	1.050	1.086
3.834	4.075	4.080	4.316	4.561	4.808	4.821	5.070	5.319	5.583	5.831
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.476	1.435	1.360	1.313	1.267	1.227	1.206	1.188	1.176	1.168	1.165
17.18	18.41	25.97	27.63	29.24	30.63	25.49	26.05	26.42	26.65	26.79
1.143	1.228	1.394	1.511	1.634	1.747	1.843	1.901	1.940	1.965	1.980
6.078	6.324	6.664	6.866	7.082	7.309	7.566	7.791	8.031	8.276	8.526
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
1.162	1.160	1.159	1.153	1.152	1.151					
26.89	26.97	27.05	31.46	31.66	32.01					
1.989	1.994	1.996	1.998	1.999	1.999					
8.774	9.023	9.273	9.529	9.779	10.030					

262 TAPS C7H17NO6S

-1	25.0	8.300	243.27									pHL	3.00	3.25	3.50
												RE	□□□□□□	□□□□□□	□□□□□□
												t	29.08	27.52	26.46
												Z	0.004	0.005	0.007
												pHS	5.946	6.034	6.115

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	□□□□□□	91.527	73.907	36.649	33.079
25.63	25.01	21.36	21.23	21.11	21.01	24.24	24.21	24.18	21.16	21.16
0.008	0.010	0.014	0.016	0.019	0.023	0.028	0.033	0.041	0.084	0.093
6.200	6.296	6.438	6.499	6.575	6.666	6.748	6.829	6.925	7.252	7.301

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
28.756	24.110	12.350	11.273	9.964	8.562	6.149	5.678	5.143	4.622	4.077
21.16	21.17	30.19	30.21	30.24	30.29	21.21	21.22	21.24	21.27	21.34
0.108	0.129	0.255	0.280	0.317	0.371	0.527	0.572	0.634	0.708	0.809
7.369	7.455	7.816	7.870	7.947	8.049	8.320	8.398	8.509	8.654	8.894

8.75	9.00	9.25	9.50	9.75	10.00
3.833	3.640	3.507	3.394	3.348	3.314
21.40	21.51	21.72	28.69	29.72	31.90
0.862	0.909	0.944	0.972	0.984	0.991
9.063	9.266	9.493	9.806	10.056	10.321

(Ref.) : 11 , 9

N-Tris(hydroxymethyl)methyl-3-aminopropanesulfonic acid

263 TARTARIC ACID (S) C4H6O6

-1	32.6	3.036	150.09									pHL	3.00	3.25	3.50
-2	60.7	4.366										RE	2.907	2.590	2.336
												t	29.86	28.25	27.62
												Z	0.878	0.997	1.120
												pHS	3.464	3.622	3.784

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.114	1.921	1.883	1.758	1.653	1.575	1.565	1.515	1.482	1.474	1.462
27.67	28.23	25.73	26.37	27.03	27.59	30.62	31.01	31.28	28.72	28.81
1.257	1.407	1.452	1.577	1.698	1.800	1.808	1.878	1.927	1.958	1.975
3.964	4.163	4.223	4.404	4.610	4.833	4.855	5.083	5.321	5.571	5.809

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.455	1.450	1.439	1.437	1.434	1.432	1.449	1.448	1.447	1.445	1.447
28.87	28.90	37.01	37.01	37.01	36.99	28.90	28.90	28.91	28.92	28.93
1.986	1.992	1.996	1.998	1.999	1.999	2.000	2.000	2.000	2.000	2.000
6.055	6.303	6.575	6.823	7.072	7.322	7.552	7.802	8.051	8.301	8.552

8.75	9.00	9.25	9.50	9.75	10.00
1.446	1.445	1.444	1.436	1.434	1.431
28.96	29.01	29.09	34.62	34.90	35.42
2.000	2.000	2.000	2.000	2.000	2.000
8.802	9.052	9.302	9.570	9.820	10.072

(Ref.) : 10 , 1

264 TARTRONIC ACID C3H4O5

-1	36.0	2.366	120.06									pHL	3.00	3.25	3.50
-2	68.3	4.735										RE	2.374	2.253	2.141
												t	27.42	25.20	24.17
												Z	0.957	1.013	1.073
												pHS	3.327	3.520	3.718

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.021	1.886	1.858	1.733	1.611	1.505	1.491	1.414	1.358	1.326	1.306
24.01	24.55	22.42	23.31	24.32	25.27	27.97	28.71	29.25	27.25	27.45
1.148	1.246	1.277	1.386	1.511	1.638	1.653	1.758	1.843	1.908	1.943
3.929	4.152	4.212	4.411	4.621	4.840	4.868	5.085	5.315	5.576	5.802

6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.292	1.283	1.272	1.268	1.266	1.264	1.276	1.275	1.274	1.273	1.274
27.58	27.66	34.83	34.85	34.86	34.86	27.72	27.73	27.73	27.74	27.75
1.967	1.981	1.989	1.994	1.997	1.998	1.999	1.999	2.000	2.000	2.000
6.042	6.288	6.554	6.800	7.048	7.298	7.535	7.785	8.034	8.284	8.535

8.75	9.00	9.25	9.50	9.75	10.00
1.274	1.273	1.272	1.266	1.264	1.263
27.77	27.81	27.88	32.73	32.96	33.37
2.000	2.000	2.000	2.000	2.000	2.000
8.785	9.035	9.285	9.546	9.796	10.047

(Ref.) : 10 , 1

265 TEREPHTHALIC ACID C8H6O4

-1	28.0	3.540	166.13				pHL	3.00	3.25	3.50
-2	53.0	4.460					RE	4.141	3.556	3.106
							t	32.28	30.69	29.94
							Z	0.716	0.843	0.976
							pHS	3.642	3.772	3.904

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.722	2.399	2.314	2.130	1.975	1.860	1.844	1.773	1.726	1.715	1.698
29.78	30.14	27.23	27.77	28.40	28.98	32.49	32.92	33.21	30.27	30.37
1.129	1.302	1.369	1.505	1.643	1.762	1.774	1.856	1.913	1.950	1.971
4.054	4.229	4.299	4.458	4.649	4.864	4.892	5.113	5.349	5.596	5.833
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.688	1.681	1.665	1.662	1.659	1.656	1.680	1.678	1.677	1.675	1.678
30.43	30.46	39.86	39.86	39.85	39.83	30.48	30.48	30.48	30.49	30.51
1.983	1.990	1.995	1.997	1.998	1.999	1.999	2.000	2.000	2.000	2.000
6.077	6.325	6.605	6.854	7.103	7.352	7.574	7.823	8.073	8.323	8.574
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 7				
1.676	1.674	1.672	1.661	1.658	1.654					
30.54	30.60	30.70	37.15	37.52	38.23					
2.000	2.000	2.000	2.000	2.000	2.000					
8.824	9.074	9.325	9.600	9.851	10.104					

266 THIOACETIC ACID C2H4OS

-1	43.7	3.337	76.11				pHL	3.00	3.25	3.50
							RE	2.925	2.617	2.393
							t	22.16	20.66	19.65
							Z	0.623	0.697	0.764
							pHS	3.521	3.665	3.812

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.216	2.080	2.059	1.987	1.933	1.897	1.893	1.873	1.860	1.859	1.855
18.91	18.41	16.46	16.22	16.06	15.95	17.91	17.86	17.82	16.02	16.01
0.827	0.882	0.895	0.928	0.955	0.973	0.974	0.985	0.991	0.995	0.997
3.979	4.174	4.227	4.408	4.620	4.851	4.874	5.110	5.354	5.595	5.838
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.852	1.849	1.845	1.844	1.843	1.842	1.850	1.850	1.849	1.848	1.850
16.00	16.00	21.24	21.24	21.24	21.24	15.97	15.97	15.98	15.99	15.99
0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.086	6.335	6.622	6.871	7.121	7.371	7.585	7.835	8.085	8.335	8.586
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
1.849	1.848	1.846	1.844	1.842	1.840					
16.02	16.05	16.12	19.75	20.00	20.46					
1.000	1.000	1.000	1.000	1.000	1.000					
8.836	9.086	9.337	9.619	9.871	10.125					

267 THIOCYANIC ACID HSCN

-1	68.5	0.848	59.09				pHL	3.00	3.25	3.50
							RE	1.166	1.163	1.161
							t	19.19	17.25	16.13
							Z	0.994	0.997	0.998
							pHS	3.050	3.290	3.531

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.160	1.159	1.160	1.160	1.160	1.159	1.159	1.159	1.159	1.160	1.160
15.49	15.12	13.96	13.75	13.63	13.57	14.79	14.76	14.74	13.61	13.60
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.775	4.023	4.024	4.270	4.518	4.767	4.771	5.021	5.271	5.518	5.767
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.159	1.159	1.159	1.159	1.159	1.159	1.160	1.160	1.160	1.159	1.160
13.60	13.60	16.88	16.88	16.88	16.88	13.58	13.58	13.58	13.59	13.59
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.017	6.267	6.525	6.775	7.025	7.275	7.517	7.767	8.017	8.267	8.517
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2				
1.159	1.159	1.159	1.159	1.159	1.158					
13.60	13.62	13.65	15.88	15.98	16.16					
1.000	1.000	1.000	1.000	1.000	1.000					
8.767	9.017	9.268	9.524	9.775	10.025					

268 THIOCYANOACETIC ACID C3H3NOS

-1	40.6	2.585	101.10

pHL	3.00	3.25	3.50
RE	2.311	2.200	2.126
t	24.38	22.14	20.70
Z	0.858	0.902	0.934
pHS	3.328	3.511	3.701

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.074	2.039	2.045	2.025	2.013	2.004	2.003	1.997	1.994	2.000	1.999
19.74	19.14	17.09	16.78	16.58	16.47	18.59	18.52	18.49	16.54	16.53
0.958	0.975	0.976	0.985	0.991	0.995	0.995	0.997	0.998	0.999	1.000
3.910	4.137	4.153	4.372	4.607	4.851	4.872	5.117	5.366	5.601	5.849
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.997	1.996	1.991	1.990	1.989	1.988	1.999	1.998	1.997	1.996	1.998
16.52	16.52	22.18	22.18	22.17	22.17	16.49	16.49	16.50	16.51	16.52
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.098	6.348	6.639	6.889	7.139	7.389	7.598	7.848	8.098	8.348	8.599
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
1.997	1.995	1.994	1.990	1.988	1.986					
16.54	16.58	16.66	20.60	20.89	21.44					
1.000	1.000	1.000	1.000	1.000	1.000					
8.850	9.100	9.351	9.637	9.890	10.145					

269 THIOGLYCOLIC ACID C2H4O2S

-1	38.6	3.545	92.11

pHL	3.00	3.25	3.50
RE	3.687	3.260	2.945
t	23.62	22.04	20.97
Z	0.560	0.635	0.704
pHS	3.619	3.753	3.888

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.687	2.483	2.441	2.332	2.247	2.188	2.181	2.147	2.125	2.123	2.115
20.18	19.63	17.39	17.14	16.96	16.85	19.07	19.01	18.97	16.92	16.91
0.773	0.839	0.858	0.899	0.934	0.960	0.962	0.977	0.987	0.992	0.996
4.044	4.226	4.289	4.456	4.657	4.881	4.910	5.141	5.383	5.622	5.863
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.110	2.107	2.100	2.099	2.097	2.095	2.108	2.107	2.106	2.104	2.106
16.91	16.90	22.87	22.86	22.86	22.86	16.87	16.87	16.88	16.89	16.90
0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.110	6.358	6.653	6.902	7.152	7.402	7.608	7.858	8.108	8.358	8.609
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.105	2.104	2.102	2.098	2.095	2.093					
16.93	16.97	17.06	21.22	21.56	22.18					
1.000	1.000	1.000	1.000	1.000	1.000					
8.859	9.110	9.361	9.650	9.903	10.159					

270 THIOSULFURIC ACID H2S2O3

-1	44.0	0.600	114.13
-2	88.1	1.720	

pHL	3.00	3.25	3.50
RE	0.986	0.979	0.974
t	35.11	31.74	29.85
Z	1.965	1.980	1.989
pHS	3.001	3.250	3.501

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
0.972	0.970	0.973	0.972	0.972	0.971	0.969	0.969	0.968	0.971	0.971
28.79	28.20	26.29	25.95	25.77	25.66	27.69	27.63	27.60	25.73	25.72
1.994	1.996	1.996	1.998	1.999	1.999	1.999	2.000	2.000	2.000	2.000
3.751	4.002	4.002	4.252	4.503	4.753	4.752	5.002	5.252	5.503	5.753
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
0.971	0.971	0.967	0.967	0.966	0.965	0.971	0.971	0.971	0.971	0.971
25.72	25.72	31.15	31.14	31.14	31.14	25.68	25.68	25.69	25.70	25.70
2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
6.003	6.253	6.501	6.751	7.001	7.251	7.503	7.753	8.003	8.253	8.503
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 4				
0.971	0.971	0.971	0.967	0.967	0.966					
25.72	25.75	25.79	29.46	29.60	29.86					
2.000	2.000	2.000	2.000	2.000	2.000					
8.753	9.003	9.253	9.501	9.751	10.001					

271 p-TOLUENESULFONIC ACID C7H8O3S

-1	31.1	-2.000	172.20				pHL	3.00	3.25	3.50
							RE	2.630	2.630	2.630
							t	29.77	26.46	24.40
							Z	1.000	1.000	1.000
							pHS	3.320	3.525	3.732

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.630	2.628	2.643	2.643	2.641	2.639	2.636	2.633	2.631	2.646	2.645
23.08	22.26	19.58	19.15	18.88	18.73	21.53	21.45	21.40	18.83	18.82
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.953	4.188	4.192	4.418	4.657	4.902	4.930	5.177	5.426	5.654	5.903
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.643	2.640	2.630	2.629	2.627	2.624	2.646	2.645	2.643	2.641	2.645
18.81	18.80	26.28	26.28	26.27	26.26	18.77	18.77	18.78	18.79	18.81
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.152	6.402	6.710	6.960	7.210	7.459	7.652	7.902	8.152	8.402	8.654
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12				
2.643	2.640	2.637	2.628	2.624	2.619					
18.85	18.92	19.05	24.39	24.95	26.05					
1.000	1.000	1.000	1.000	1.000	1.000					
8.905	9.156	9.407	9.712	9.968	10.229					

272 m-TOLUIC ACID C8H8O2

-1	29.1	4.272	136.15				pHL	3.00	3.25	3.50
							RE	8.002	6.822	5.932
							t	27.47	25.75	24.58
							Z	0.340	0.400	0.462
							pHS	3.962	4.072	4.180

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.166	4.499	4.188	3.854	3.545	3.292	3.240	3.085	2.977	2.928	2.891
23.69	23.05	19.96	19.73	19.53	19.40	22.38	22.30	22.26	19.52	19.50
0.532	0.614	0.666	0.725	0.791	0.854	0.867	0.911	0.945	0.968	0.981
4.301	4.445	4.540	4.661	4.816	5.003	5.051	5.250	5.472	5.716	5.938
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.866	2.850	2.828	2.823	2.819	2.815	2.840	2.839	2.836	2.833	2.838
19.49	19.48	27.51	27.50	27.49	27.48	19.45	19.45	19.46	19.47	19.50
0.989	0.994	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.176	6.421	6.734	6.981	7.229	7.479	7.668	7.917	8.167	8.417	8.670
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.835	2.832	2.828	2.817	2.813	2.806					
19.54	19.63	19.77	25.54	26.21	27.55					
1.000	1.000	1.000	1.000	1.000	1.000					
8.920	9.171	9.423	9.733	9.990	10.253					

273 o-TOLUIC ACID C8H8O2

-1	29.1	3.908	136.15				pHL	3.00	3.25	3.50
							RE	6.018	5.231	4.638
							t	28.03	26.09	24.78
							Z	0.456	0.527	0.596
							pHS	3.806	3.927	4.048

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.138	3.719	3.598	3.378	3.190	3.051	3.027	2.945	2.891	2.880	2.861
23.80	23.10	20.06	19.77	19.55	19.40	22.39	22.31	22.26	19.52	19.50
0.670	0.748	0.780	0.832	0.883	0.925	0.931	0.957	0.975	0.985	0.991
4.186	4.350	4.423	4.569	4.750	4.960	5.000	5.221	5.456	5.691	5.927
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.849	2.840	2.823	2.820	2.817	2.814	2.840	2.838	2.836	2.833	2.837
19.49	19.48	27.51	27.50	27.49	27.48	19.45	19.45	19.46	19.47	19.50
0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.171	6.419	6.732	6.980	7.229	7.479	7.667	7.917	8.167	8.417	8.670
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.835	2.832	2.828	2.817	2.813	2.806					
19.54	19.63	19.77	25.54	26.21	27.55					
1.000	1.000	1.000	1.000	1.000	1.000					
8.920	9.171	9.423	9.733	9.990	10.253					

274 p-TOLUIC ACID C8H8O2

-1	29.1	4.373	136.15							
							pHL	3.00	3.25	3.50
							RE	8.717	7.400	6.406
							t	27.34	25.67	24.53
							Z	0.312	0.368	0.427
							pHS	4.007	4.115	4.220

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.547	4.794	4.406	4.035	3.685	3.392	3.327	3.145	3.015	2.949	2.904
23.67	23.03	19.93	19.71	19.53	19.40	22.37	22.30	22.26	19.52	19.50
0.495	0.575	0.631	0.691	0.759	0.827	0.843	0.893	0.933	0.961	0.976
4.337	4.476	4.576	4.692	4.839	5.019	5.070	5.262	5.479	5.727	5.943
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.874	2.855	2.830	2.824	2.819	2.815	2.841	2.839	2.836	2.833	2.838
19.49	19.48	27.50	27.50	27.49	27.48	19.45	19.45	19.46	19.47	19.50
0.986	0.992	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.178	6.422	6.736	6.981	7.230	7.479	7.668	7.917	8.167	8.417	8.670
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 1				
2.835	2.832	2.828	2.817	2.813	2.806					
19.54	19.63	19.77	25.54	26.21	27.55					
1.000	1.000	1.000	1.000	1.000	1.000					
8.920	9.171	9.423	9.733	9.990	10.253					

275 TRIBROMOACETIC ACID C2HBr3O2

-1	36.5	1.000	296.74							
							pHL	3.00	3.25	3.50
							RE	2.235	2.231	2.228
							t	26.84	23.91	22.11
							Z	0.995	0.997	0.998
							pHS	3.264	3.474	3.686
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.226	2.225	2.234	2.233	2.232	2.230	2.228	2.227	2.225	2.235	2.234
20.97	20.28	18.02	17.64	17.42	17.29	19.66	19.59	19.55	17.37	17.36
0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.911	4.148	4.152	4.382	4.623	4.869	4.892	5.139	5.388	5.620	5.869
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.233	2.231	2.224	2.224	2.222	2.221	2.235	2.234	2.233	2.231	2.234
17.35	17.35	23.68	23.67	23.67	23.66	17.32	17.32	17.33	17.34	17.35
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.119	6.368	6.666	6.916	7.166	7.416	7.619	7.869	8.119	8.369	8.620
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12				
2.233	2.231	2.229	2.223	2.221	2.218					
17.38	17.43	17.52	21.96	22.34	23.06					
1.000	1.000	1.000	1.000	1.000	1.000					
8.870	9.121	9.372	9.665	9.919	10.176					

276 TRICHLOROACETIC ACID C2HCl3O2

-1	37.9	0.635	163.39							
							pHL	3.00	3.25	3.50
							RE	2.144	2.142	2.141
							t	26.25	23.39	21.63
							Z	0.998	0.999	0.999
							pHS	3.249	3.461	3.675
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.139	2.138	2.147	2.146	2.145	2.144	2.142	2.141	2.139	2.148	2.147
20.53	19.86	17.69	17.33	17.11	16.99	19.27	19.20	19.16	17.07	17.06
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.901	4.139	4.143	4.373	4.615	4.862	4.883	5.131	5.380	5.613	5.862
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.146	2.145	2.139	2.138	2.137	2.135	2.148	2.148	2.146	2.145	2.147
17.05	17.05	23.13	23.12	23.12	23.12	17.01	17.02	17.02	17.03	17.04
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.111	6.361	6.657	6.906	7.156	7.406	7.611	7.861	8.111	8.361	8.613
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 2 , 7				
2.146	2.144	2.143	2.138	2.136	2.133					
17.07	17.12	17.21	21.46	21.81	22.46					
1.000	1.000	1.000	1.000	1.000	1.000					
8.863	9.113	9.364	9.655	9.909	10.165					

277 TRICHLOROACRYLIC ACID C3HCl3O2 175.40

-1	33.4	0.000					pHL	3.00	3.25	3.50
							RE	2.442	2.441	2.441
							t	28.41	25.28	23.33
							Z	1.000	1.000	1.000
							pHS	3.294	3.501	3.711

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.440	2.439	2.452	2.451	2.450	2.448	2.445	2.443	2.441	2.454	2.453
22.09	21.34	18.85	18.44	18.20	18.06	20.66	20.58	20.53	18.15	18.14
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
3.934	4.169	4.173	4.401	4.641	4.887	4.913	5.160	5.409	5.639	5.887
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.451	2.449	2.441	2.439	2.438	2.436	2.454	2.453	2.451	2.450	2.453
18.13	18.12	25.06	25.06	25.05	25.05	18.09	18.09	18.10	18.11	18.13
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.137	6.387	6.690	6.940	7.190	7.440	7.637	7.887	8.137	8.387	8.639
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 12				
2.451	2.449	2.446	2.439	2.436	2.432					
18.16	18.22	18.33	23.25	23.72	24.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.889	9.140	9.391	9.691	9.945	10.204					

278 TRICHLOROLACTIC ACID C3H3Cl3O3 193.41

-1	34.2	2.347					pHL	3.00	3.25	3.50
							RE	2.595	2.519	2.469
							t	27.48	24.70	22.93
							Z	0.915	0.943	0.963
							pHS	3.343	3.533	3.728

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.434	2.411	2.422	2.409	2.400	2.394	2.391	2.387	2.383	2.395	2.393
21.77	21.04	18.60	18.22	17.98	17.84	20.38	20.30	20.26	17.94	17.92
0.977	0.986	0.987	0.992	0.995	0.997	0.997	0.999	0.999	1.000	1.000
3.941	4.171	4.181	4.402	4.639	4.884	4.909	5.155	5.403	5.634	5.883
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.391	2.389	2.381	2.380	2.378	2.376	2.394	2.393	2.391	2.389	2.392
17.91	17.91	24.68	24.68	24.67	24.67	17.87	17.88	17.88	17.90	17.91
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.132	6.382	6.684	6.934	7.183	7.433	7.632	7.882	8.132	8.382	8.634
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.391	2.389	2.386	2.380	2.377	2.372					
17.95	18.00	18.11	22.89	23.33	24.18					
1.000	1.000	1.000	1.000	1.000	1.000					
8.884	9.135	9.386	9.684	9.938	10.197					

279 TRIMETAPHOSPHORIC ACID H3P3O9 239.94

-1	28.9	-2.000					pHL	3.00	3.25	3.50
-2	57.8	-1.000					RE	1.088	1.081	1.075
-3	87.6	2.050					t	54.45	49.14	46.13
							Z	2.946	2.969	2.982
							pHS	3.029	3.275	3.522

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
1.072	1.069	1.080	1.078	1.077	1.076	1.070	1.068	1.067	1.078	1.077
44.42	43.45	40.37	39.82	39.50	39.33	42.66	42.56	42.49	39.47	39.45
2.990	2.994	2.994	2.997	2.998	2.999	2.999	2.999	3.000	3.000	3.000
3.771	4.020	4.021	4.269	4.519	4.769	4.770	5.020	5.270	5.519	5.769
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
1.076	1.075	1.064	1.063	1.061	1.059	1.078	1.078	1.077	1.076	1.077
39.44	39.43	48.34	48.32	48.29	48.26	39.39	39.39	39.39	39.40	39.41
3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
6.019	6.269	6.522	6.772	7.021	7.271	7.519	7.769	8.019	8.269	8.519
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 4				
1.077	1.075	1.074	1.064	1.062	1.061					
39.44	39.48	39.55	45.57	45.80	46.24					
3.000	3.000	3.000	3.000	3.000	3.000					
8.769	9.019	9.269	9.521	9.771	10.021					

280 TRIMETHYLACETIC ACID (S) C5H10O2

-1 31.8 5.037 102.13

pHL	3.00	3.25	3.50
RE	15.015	12.497	10.607
t	25.11	23.83	22.96
Z	0.163	0.196	0.231
pHS	4.309	4.406	4.497

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
8.954	7.461	6.196	5.549	4.883	4.256	4.014	3.610	3.265	2.947	2.833
22.28	21.76	18.88	18.74	18.61	18.51	21.18	21.13	21.10	18.61	18.60
0.275	0.331	0.403	0.451	0.515	0.593	0.630	0.702	0.779	0.872	0.908
4.596	4.710	4.841	4.926	5.034	5.170	5.237	5.378	5.550	5.834	5.995
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.738	2.672	2.615	2.595	2.581	2.573	2.590	2.587	2.584	2.581	2.584
18.59	18.59	25.89	25.88	25.88	25.87	18.55	18.55	18.56	18.57	18.59
0.940	0.963	0.982	0.989	0.994	0.997	0.998	0.999	0.999	1.000	1.000
6.195	6.420	6.735	6.966	7.209	7.456	7.651	7.899	8.148	8.398	8.650
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 7				
2.582	2.579	2.576	2.568	2.564	2.559					
18.63	18.70	18.82	24.02	24.55	25.59					
1.000	1.000	1.000	1.000	1.000	1.000					
8.900	9.151	9.402	9.705	9.961	10.221					

281 TRIMETHYLACRYLIC ACID C6H10O2

-1 30.3 4.420 114.14

pHL	3.00	3.25	3.50
RE	8.773	7.431	6.419
t	26.51	24.94	23.88
Z	0.297	0.351	0.408
pHS	4.023	4.131	4.234

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
5.543	4.772	4.344	3.971	3.614	3.310	3.240	3.051	2.914	2.838	2.791
23.06	22.47	19.48	19.28	19.11	18.98	21.83	21.76	21.72	19.09	19.08
0.474	0.553	0.613	0.673	0.742	0.812	0.829	0.882	0.925	0.956	0.973
4.349	4.484	4.590	4.701	4.845	5.020	5.072	5.259	5.473	5.725	5.937
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.759	2.738	2.714	2.708	2.703	2.699	2.722	2.720	2.718	2.715	2.719
19.07	19.06	26.75	26.74	26.74	26.73	19.03	19.03	19.04	19.05	19.07
0.984	0.991	0.995	0.997	0.999	0.999	0.999	1.000	1.000	1.000	1.000
6.170	6.413	6.725	6.970	7.218	7.467	7.659	7.908	8.158	8.408	8.660
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.717	2.714	2.710	2.701	2.696	2.691					
19.12	19.19	19.32	24.83	25.43	26.62					
1.000	1.000	1.000	1.000	1.000	1.000					
8.911	9.162	9.413	9.720	9.976	10.238					

282 2.4.6-TRIMETHYLBENZOIC ACID C10H12O2

-1 24.7 3.437 164.20

pHL	3.00	3.25	3.50
RE	5.123	4.630	4.265
t	32.68	29.90	28.02
Z	0.643	0.713	0.777
pHS	3.664	3.804	3.948

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
3.971	3.746	3.739	3.613	3.518	3.455	3.440	3.403	3.380	3.395	3.386
26.67	25.75	22.23	21.80	21.50	21.31	24.88	24.77	24.70	21.45	21.43
0.837	0.889	0.898	0.930	0.956	0.974	0.976	0.986	0.992	0.995	0.997
4.115	4.309	4.348	4.529	4.740	4.971	5.009	5.246	5.490	5.716	5.960
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.380	3.374	3.351	3.349	3.345	3.342	3.381	3.379	3.375	3.371	3.378
21.41	21.40	30.93	30.92	30.91	30.90	21.37	21.37	21.38	21.40	21.44
0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.208	6.457	6.779	7.028	7.278	7.528	7.707	7.957	8.207	8.457	8.710
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 7				
3.374	3.370	3.364	3.346	3.339	3.328					
21.50	21.62	21.83	28.87	29.94	32.19					
1.000	1.000	1.000	1.000	1.000	1.000					
8.961	9.212	9.465	9.790	10.050	10.320					

283 TRIMETYLPYRUVIC ACID C6H1003
-1 29.2 1.469 130.14

pHL	3.00	3.25	3.50
RE	2.842	2.830	2.823
t	30.97	27.56	25.41
Z	0.988	0.992	0.995
pHS	3.351	3.551	3.754

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.817	2.813	2.830	2.828	2.825	2.822	2.817	2.814	2.811	2.829	2.828
24.01	23.15	20.28	19.82	19.54	19.37	22.37	22.27	22.22	19.48	19.46
0.997	0.998	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
3.972	4.205	4.210	4.434	4.672	4.917	4.946	5.193	5.442	5.669	5.917
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.825	2.822	2.809	2.808	2.806	2.803	2.829	2.828	2.826	2.823	2.827
19.45	19.45	27.44	27.43	27.43	27.42	19.41	19.42	19.42	19.44	19.46
1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.166	6.416	6.728	6.978	7.228	7.477	7.666	7.916	8.166	8.416	8.669
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.825	2.822	2.818	2.807	2.803	2.796					
19.51	19.59	19.73	25.48	26.15	27.47					
1.000	1.000	1.000	1.000	1.000	1.000					
8.919	9.170	9.422	9.732	9.989	10.252					

284 VALERIC ACID C5H1002
-1 31.6 4.842 102.13

pHL	3.00	3.25	3.50
RE	12.475	10.427	8.888
t	25.35	24.02	23.10
Z	0.198	0.237	0.279
pHS	4.216	4.316	4.410

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
7.545	6.338	5.413	4.873	4.326	3.823	3.657	3.333	3.070	2.860	2.771
22.39	21.86	18.97	18.82	18.68	18.57	21.27	21.22	21.18	18.67	18.66
0.330	0.395	0.467	0.520	0.588	0.667	0.698	0.768	0.836	0.906	0.936
4.512	4.632	4.757	4.848	4.966	5.112	5.175	5.329	5.516	5.788	5.967
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.703	2.657	2.616	2.602	2.593	2.586	2.606	2.603	2.600	2.598	2.601
18.65	18.65	26.00	25.99	25.99	25.98	18.61	18.61	18.62	18.63	18.65
0.960	0.976	0.988	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000
6.180	6.413	6.726	6.963	7.209	7.456	7.651	7.900	8.149	8.399	8.651
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 10 , 1				
2.599	2.596	2.593	2.585	2.581	2.576					
18.69	18.76	18.88	24.12	24.66	25.72					
1.000	1.000	1.000	1.000	1.000	1.000					
8.901	9.152	9.404	9.707	9.963	10.223					

285 VANILLIC ACID C8H804
-1 27.1 4.523 168.15

pHL	3.00	3.25	3.50
RE	10.559	8.918	7.677
t	28.62	26.85	25.64
Z	0.276	0.328	0.382
pHS	4.084	4.189	4.291

3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
6.601	5.651	5.121	4.658	4.213	3.830	3.734	3.494	3.317	3.218	3.156
24.73	24.06	20.72	20.49	20.31	20.17	23.37	23.30	23.25	20.31	20.29
0.446	0.523	0.583	0.643	0.714	0.788	0.808	0.865	0.913	0.949	0.968
4.404	4.537	4.640	4.749	4.889	5.060	5.114	5.298	5.508	5.758	5.967
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
3.114	3.087	3.054	3.046	3.039	3.034	3.064	3.062	3.059	3.055	3.060
20.28	20.27	28.92	28.91	28.90	28.89	20.24	20.24	20.25	20.27	20.30
0.981	0.989	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000
6.198	6.440	6.759	7.003	7.251	7.500	7.685	7.934	8.184	8.434	8.687
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 11 , 2				
3.057	3.054	3.049	3.036	3.030	3.022					
20.35	20.44	20.61	26.90	27.72	29.38					
1.000	1.000	1.000	1.000	1.000	1.000					
8.937	9.188	9.441	9.757	10.015	10.281					

286 VINYLACETIC ACID C4H6O2

-1	38.6	4.342	86.09				pHL	3.00	3.25	3.50
							RE	6.648	5.639	4.882
							t	22.58	21.44	20.66
							Z	0.306	0.361	0.418
							pHS	3.962	4.070	4.173
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
4.227	3.649	3.297	3.026	2.765	2.542	2.494	2.355	2.254	2.193	2.159
20.04	19.58	17.24	17.09	16.95	16.85	19.06	19.01	18.97	16.92	16.91
0.485	0.563	0.629	0.686	0.753	0.821	0.837	0.888	0.928	0.959	0.975
4.287	4.423	4.538	4.648	4.791	4.967	5.016	5.202	5.416	5.675	5.887
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.136	2.121	2.107	2.103	2.099	2.097	2.108	2.107	2.106	2.104	2.107
16.91	16.90	22.87	22.86	22.86	22.86	16.87	16.87	16.88	16.89	16.90
0.985	0.991	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000
6.120	6.363	6.660	6.905	7.153	7.402	7.609	7.858	8.108	8.358	8.609
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3 , 7				
2.105	2.104	2.102	2.098	2.095	2.093					
16.93	16.97	17.06	21.22	21.56	22.18					
1.000	1.000	1.000	1.000	1.000	1.000					
8.859	9.110	9.361	9.650	9.903	10.159					

287 VINYLGLYCOLIC ACID C4H6O3

-1	35.4	3.319	102.09				pHL	3.00	3.25	3.50
							RE	3.499	3.155	2.903
							t	25.41	23.48	22.18
							Z	0.648	0.720	0.784
							pHS	3.552	3.696	3.845
3.75	4.00	4.00	4.25	4.50	4.75	4.75	5.00	5.25	5.50	5.75
2.704	2.554	2.540	2.458	2.397	2.357	2.352	2.328	2.314	2.318	2.313
21.24	20.61	18.18	17.88	17.68	17.55	19.99	19.92	19.88	17.63	17.62
0.844	0.895	0.904	0.935	0.960	0.976	0.977	0.987	0.992	0.996	0.997
4.016	4.213	4.257	4.442	4.656	4.889	4.917	5.154	5.399	5.634	5.878
6.00	6.25	6.50	6.75	7.00	7.25	7.50	7.75	8.00	8.25	8.50
2.309	2.306	2.298	2.296	2.295	2.293	2.308	2.307	2.306	2.304	2.307
17.61	17.61	24.14	24.14	24.13	24.13	17.57	17.58	17.58	17.59	17.61
0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
6.126	6.375	6.675	6.925	7.174	7.424	7.625	7.875	8.125	8.375	8.626
8.75	9.00	9.25	9.50	9.75	10.00	(Ref.) : 3				
2.305	2.304	2.301	2.296	2.293	2.289					
17.64	17.70	17.79	22.39	22.80	23.57					
1.000	1.000	1.000	1.000	1.000	1.000					
8.877	9.127	9.379	9.674	9.928	10.186					

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11 Unpublished data obtained in our laboratory.
12 Assumed values.

PUBLICATION SCHEDULE FOR 1983

Journal of Chromatography (incorporating *Chromatographic Reviews*) and *Journal of Chromatography, Biomedical Applications*

MONTH	D 1982	J	F	M	A	M	J	
Journal of Chromatography	252 253/1 253/2	254 255 256/1	256/2 256/3 257/1	257/2 258 259/1	259/2 259/3 260/1	260/2 261/1 261/2	261/3 262 263	The publication schedule for further issues will be published later.
Chromatographic Reviews					271/1		271/2	
Biomedical Applications		272/1	272/2	273/1	273/2	274	275/1	

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