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CRITICAL COMPILATION OF SCALES OF SOLVENT PARAMETERS. PART I. PURE, NON-HYDROGEN BOND DONOR SOLVENTS

(Technical Report)

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INTRODUCTION AND FUNDAMENTAL CONCEPTS

It has long been known [1] that solvents often affect chemical reactivity, this involving, e.g. the shift of the position of chemical equilibria (thermodynamic aspect) as well as significant changes in reaction rate constants (kinetic aspect). Physical properties, particularly the frequencies and intensities of transitions in IR, UV-visible, fluorescence, NMR and ESR spectroscopies are also known to be affected by solvents.

These phenomena are consequences of differences in the solvation of reagents and products (thermodynamic effects) or reagents and activated complexes (kinetic effects). Differential solvation of species in the ground and excited states accounts for the spectral phenomenology indicated above [1,2]. Differences in solvation of a given solute in two different solvents determine the size of the corresponding partition coefficient.

It is customary to state that these effects reflect the influence of 'solvent polarity'. According to Reichardt [1a] 'solvent polarity' is 'the overall solvation capability (or solvation power) of solvents, which in turn depends on the action of all possible, nonspecific and specific intermolecular interactions between solute ions or molecules and solvent molecules, excluding, however, those interactions leading to definite chemical alterations of the ions or molecules of the solute (such as protonation, oxidation, reduction, chemical complex formation, etc.)'.

This definition underscores the extreme complexity of 'solvation effects' at the molecular level. This notwithstanding, solvent effects (SE) often display some remarkable regularities that allow in many cases an 'empirical treatment' that sheds light on their origin and main contributors.

Consider a solute Σ and two different properties P_1 and P_2, taking the values $\{P_{10}, P_{11}, \ldots, P_{1i}, \ldots\}$ and $\{P_{20}, P_{21}, \ldots, P_{2i}, \ldots\}$, respectively, in solvents $S_0, S_1, \ldots, S_i, \ldots$. A scale of SEs is simply constructed by taking for each solvent, S_i, the difference $P_{1i}-P_{10}$, S_0 being chosen as a reference solvent. If the property P_1 is a 'good descriptor' of SEs on P_2, eqn 1 holds for solvent S_i:

$$P_{2i} - P_{20} = k(P_{1i} - P_{10}) \tag{1}$$

or

$$P_{2i} - P_{20} = k\,p_i \tag{2}$$

wherein k is a constant independent of the solvents and determined solely by P_2. p_i is the 'solvent parameter' characteristic of solvent S_i.

More generally, the properties being compared might belong to two different solutes.

For any property P_m of any solute, and if P_1 is a 'good descriptor', eqn 3 holds:

$$P_{mi} - P_{m0} = k_m\,p_i \tag{3}$$

We draw attention to the (frequently overlooked) fact that if equations such as (3) were truly general, then, all SEs would be linearly related to an extremely high degree of precision and a single, universal scale of SEs would exist. This is against all the available experimental evidence. Excellent correlations of narrower scope do exist however, that successfully link a very large amount of experimental data for a substantial variety of solvents and solutes and a relatively small number of empirical scales.

In this compilation, scales are selected on the basis of criteria to be discussed below. For each of them, the most reliable values of solvent parameters are given. The physical foundations and the scope of the scales are discussed. Some suggestions regarding their use are made. For the purpose of facilitating future work in the field, some indications are given regarding the experimental determination of the various parameters.

Solvent–solute interactions always involve dispersion or London's forces [3–6] and, very often, dipolar and/or multipolar interactions [7,8]. Current theoretical models including London's, Hildebrand's [9–11] and/or reaction field (RF) [8,12] theories allow to express these 'non-specific' parts of SEs as functions of physical properties such as the refractive index, relative permittivity and thermodynamic properties of the solvent.

Quantitative rankings of solvents ('solvent scales') can thus be constructed on the basis of such properties as the refractive index, n; electric permittivity (formerly known as dielectric constant), ε_r; Hildebrand's solubility parameter, δ_H; the modulus of the molecular dipole moment, μ, and various functions thereof. These scales shall be termed 'model-independent'. Quite generally, it is assumed that dispersive and electrostatic interactions are independent and additive. Following Palm and Koppel, [13,14] it is further assumed that other contributions to solvent–solute interactions, notably hydrogen bonding are also independent from and additive to, the 'non-specific' contributions.

Use is often made of 'model-dependent' scales. They are based on **the similarity principle** [15]: the ranking of the efficiency of solvents on a given property is quantitatively compared to their influence on a **reference** physical or chemical property of a **reference solute** ('molecular probe'). The associated formalism is quite simple and has been outlined above. These scales can be divided into two different categories, depending on whether they quantify the overall 'polarity effect' of the solvent, in Reichardt's sense or else, they are intended to measure one or various components of the overall solvation power of the solvent.

Some scales have been built on the basis of a statistical treatment of SEs on large sets of experimental data of various origins. They are absolutely 'empirical' in that they try to quantify 'average' SEs without specifically seeking a formal link with current theoretical concepts on solvent–solute interactions.

Last we mention that the case of self-associated solvents and mixtures thereof involves a number of conceptual and experimental difficulties that, in our opinion, justify a separate treatment.

Here we deal with nonhydrogen bond donor solvents, although a number of weak hydrogen bond donor solvents are also included.

Part I of this compilation is organized as follows:

- Description of the Tables.
- Physical properties and model-independent scales.
- Table 1.
- Model-dependent scales:
- (a) 'Overall solvation' scales.
- (b) Scales of dipolarity/polarizability.
- (c) Scales of hydrogen bonding accepting power (hydrogen bonding basicity).
- (d) Scales of 'hard' and 'soft' Lewis acidity and basicity.
- Statistical scales.
- Table 2.
- General comments on the scales.

DESCRIPTION OF THE TABLES

Data are presented for 346 solvents and the gas phase. For each of them, the Chemical Abstracts Registry Number as well as the official (IUPAC) and eventually, common names are given, together with the values for the following physical properties: refractive index (n), relative permittivity (ε_r), modulus of the molecular dipole moment (μ) and functions thereof, molar weight (M), density at 25.0 °C (d^{25}), molar volume at 25.0 °C (V_m), standard molar vaporization enthalpies and energies at 298.15 K, $\Delta_{vap}H°$ and $\Delta_{vap}U°$, and Hildebrand's solubility parameter (δ_H). Model-dependent scales are given next. These scales are based on data obtained by physical methods. In all instances the original data, e.g. IR or UV-visible

frequencies of absorption maxima are given in the original units and/or in energy units. The importance of this point has been particularly emphasized by Kosower [16]. 'Normalized values' are also given when available. In cases wherein scales are constructed using experimental data for several indicators or molecular probes, both the actual data and the averaged parameters are given for each indicator. This is intended to avoid blurring any specific solute-dependent effects, however, small [17]. 'Single parameter scales' giving an overall quantification of SEs according to Reichardt's concept are given first. They are followed by several specific scales of 'dipolarity-polarizability' effects, hydrogen-bonding basicity and Lewis' 'hard' and 'soft' acidity and basicity. Last, representative 'statistical' scales intended to quantify general or specific solvent effects are presented.

It should be kept in mind that this is only a compilation of scales of parameters of solvent effects, that is, a tool. In no case is this work intended to be a monograph on solvent effects or even on scales of solvent effects. The final choice of the magnitudes and scales to be tabulated was made taking into consideration the advice of the various members of the working party. Because of space limitations, not all their suggestions could be followed.

The choice of the scales given in this compilation is, by its very nature, somewhat arbitrary and oversights are therefore possible. Our main guidelines were as follows:

1   The compilation had to present those physical data known to be of primary importance in most current theoretical models and correlation analysis treatments of solvent effects.

2   All empirical scales widely used over the years as well as others, however recent, that provide data for large sets of solvents had to be included.

3   As regards specific scales, as many well-identified solvent–solute interactions as possible had to be covered. For each of these scales, the criteria of widespread use and potential usefulness were taken into consideration.

4   *In general, simple physical properties of the bulk solvents and parameters determined by means of standard physical techniques or based on readily available data were preferred.*

DEFINITION, UNITS AND SOURCES OF PHYSICAL PROPERTIES AND MODEL-INDEPENDENT SCALES.

Physical properties

Symbols and units are taken from the Second Edition of the IUPAC manual on *Quantities, Units and Symbols in Physical Chemistry* [18]. The main sources of information are: (i) the Beilstein database [19] and the original publications reported therein; (ii) the fourth edition of Riddick, Bunger & Sakano's *Organic Solvents. Physical Properties and Methods of Purification* [20], (iii) the three volumes of McClellan's *Tables of Experimental Dipole Moments* [21–23], (iv) the 1994 review by Laurence, Abboud and co-workers [17a] and the Doctoral Thesis of M. T. Dalati [17b], (v) Majer & Svoboda's *Enthalpies of Vaporization of Organic Compounds. A critical review and data compilation* [24]. The values reported in the present tabulation have been averaged over the available experimental data whenever values from different sources and seemingly comparable quality were at hand.

The refractive index

The refractive index n is the ratio of the velocity of light in the vacuum to the velocity of light in a particular substance [25]. It is a dimensionless magnitude. In this compilation, refractive indexes are for the sodium-D doublet (average vacuum wavelength 589.6 nm) whenever possible. If not, values for 'white light' are given. In view of this, refractive indexes are labeled n instead of n_D. Because of the availability of data, a standard temperature of 20.0 °C was selected. When necessary, the value was obtained by interpolation from data at other temperatures. Notice that in general, refractive indexes can be experimentally determined to within 2×10^{-4} to 2×10^{-5}. In fact, when comparing data for the same solvent, at the same temperature and wavelength as determined by different groups, differences one hundred to one thousand times this value are found. Under the circumstances, n-values are consistently given here with four significant figures.

The relative permittivity (formerly known as dielectric constant)

The relative permittivity, ε_r, is a measure of the effect a solvent has on the force with which two oppositely charged plates attract each other. The reference is the attraction in vacuum. ε_r is dimensionless. Experimental values are also given at 20.0 °C. When necessary and warranted by the availability of data at other temperatures, the value at 20.0 °C was determined by interpolation. In principle, ε_r values can be determined experimentally to within 0.001. However, here again, and whenever comparisons can be carried out, the agreement between data from different laboratories is often much worse: in the range 0.01–0.1. Notice that [17a] and [17b] report one of the largest sets of ε_r values determined in the same laboratory.

Modulus of the molecular dipole moment, μ

Given a distribution of electric charges Q_i, r_i being the corresponding distance vectors to a reference point, $\mu = \Sigma Q_i r_i$ [26]. The SI unit is C m. In practice, use is often made of the debye unit, D. $1D = 3.33564 \times 10^{-30}$ C m. It is unfortunate that no homogeneous set of physical state and experimental methods could be found that applies to all the solvents of this compilation. Under the circumstances, values determined in the gas phase, particularly by microwave spectroscopy were preferred. In the absence of gas phase data, values for solutions in hexane, cyclohexane, tetrachloromethane and benzene (in this order) were chosen. Even in the gas phase, disagreements between values determined by different groups by nonspectroscopic methods are substantial, often in the 0.1–0.2 D range. As regards solution values, even larger discrepancies are not uncommon. Whenever the solute is made out of molecules involved in conformational equilibria (as in the case of 1,2-dichloroethane, $ClCH_2$-CH_2Cl) temperature and/or medium can strongly affect the value of the observed dipole moment. In these cases, the use of this magnitude for the quantitative treatment of medium effects cannot be encouraged.

Functions of n and ε_r

The use of these functions is based on fundamental concepts of reaction field (RF) [8,12] theory as applied to electrostatic and dispersive interactions. f(n) and g(r) are defined through eqns (4) and (5):

$$f(n) = (n^2 - 1)/(n^2 + 1) \tag{4}$$
$$g(\varepsilon_r) = (\varepsilon_r - 1)/(\varepsilon_r + 1) \tag{5}$$

These and cognate functions are widely used in Correlation Analysis treatments of medium effects. Let δn, $\delta \varepsilon_r$, δf and δg stand for the estimated uncertainties on n, ε_r, $f(n)$ and $g(\varepsilon_r)$. Equations 6a and 6b are readily derived from eqns 4 and 5.

$$\delta f(n)/f(n) \sim (4n\delta n)/(n^2 + 1)(n^2 - 1) \tag{6a}$$
$$\delta g(\varepsilon_r)/g(\varepsilon_r) \sim (2\delta\varepsilon_r)/(\varepsilon_r + 1)(\varepsilon_r - 1) \tag{6b}$$

In view of the orders of magnitude of n, ε_r, δn and $\delta\varepsilon_r$, eqns 6a and 6b yield estimates of $\delta f(n)/f(n)$ and $\delta g(\varepsilon_r)/g(\varepsilon_r)$ of $\sim 1-2\times10^{-3}$. Values of $f(n)$ and $g(\varepsilon_r)$ are thus given with three decimal figures. The difference $[g(\varepsilon_r) - f(n)]$ has also a theoretical foundation and is related to orientation polarization. For molecules devoid of a permanent dipole moment, Maxwell's equation, $\varepsilon_r = n^2$, holds. This expression involves the value of the refractive index extrapolated to a frequency such that no orientation polarization occurs any longer but, nevertheless low enough to include the contributions of the electronic and atomic polarizations [27]. The values of the refractive index given here are not extrapolated and therefore small differences, in the range 0.01–0.02 cannot be considered significant.

Relative density at 25 °C [28]

The relative density at 25 °C (d^{25}) is defined as the ratio of the density (mass density) of the solvent at 25 °C to that of water at 4 °C. It is a dimensionless quantity.

Molar mass [29]

The molar mass, M is defined as $M = m/n$. m is the mass of a sample, and n is the amount $n = N/L$ where N is the number of atoms or molecules and L is the Avogadro–Loschmidt constant. The SI unit is kg/mol. In this compilation, for practical reasons, values are given in g/mol.

Molar volume at 25 °C [29]

The molar volume at 25 °C ($V_m{}^{25}$) [29] is defined as the volume of one mole of the liquid at 25 °C. SI units are m^3/mol. For practical reasons, values are given in cm^3/mol.

Standard molar enthalpy of vaporization at 298.15 K

The standard molar enthalpy of vaporization at 298.15 K is noted $\Delta_{vap}H°$. It has been defined as the difference between the molar enthalpy of the ideal gas at a standard pressure and that of the saturated liquid at 298.15 K. [30] $\Delta_{vap}H°$ is given by eqn 7:

$$\Delta_{vap}H° = H°(g) - H(I, \ p_{sat}) = \Delta_{vap}H - \int_0^{p_{sat}} [V^g - T(\partial V^g / \partial T)_p] dp \tag{7}$$

The selected standard pressure is 10^5 Pa or 0.1 MPa. As indicated in [30], the enthalpy and internal energy of an ideal gas are pressure-independent and the choice of the standard state has no influence on $\Delta_{vap}H°$ values. $\Delta_{vap}H$ stands for the enthalpy of vaporization of the liquid at the reference temperature and is defined as the difference between the enthalpies of the vapor and liquid phases at this temperature and at the corresponding saturated vapor pressure, p_{sat}, eqn 8:

$$\Delta_{vap}H = H(g, p_{sat}) - H(l, p_{sat}) \tag{8}$$

$\Delta_{vap}H°$ can be written as in eqn 12:

$$\Delta_{vap}H° = \Delta_{vap}H + [H°(g) - H(g, p_{sat})] \tag{9}$$

The last term in eqn 9 is the standard departure function representing the difference between the enthalpies of the ideal gas and the saturated vapor. This term is always positive and increases with the temperature. According to [24], at temperatures more than 100 °C below the boiling point this term is always less than 0.1% of $\Delta_{vap}H$ and can be generally neglected.

Both terms in eqn 9 contribute to the overall uncertainty on $\Delta_{vap}H°$. The uncertainty on $\Delta_{vap}H$ is that associated with the experimental determination of this quantity. In general, it is in the range 0.1–3 kJ/mol. The uncertainty on the second term, whenever significant (see above) originates in the ancillary PVT information needed to carry out the pressure correction as well as on the type of compound and the method used to compute the correction. According to a comparative study by Majer & Svoboda [30], for a given compound the uncertainty increases with the temperature but is essentially independent of the method. Except for extremely volatile solvents, the leading source of uncertainty for the majority of the materials considered in this compilation is that originating in $\Delta_{vap}H$.

$\Delta_{vap}H°$ values are defined as the standard molar enthalpies of vaporization at 298.15 K. The data presented here were taken from [24] whenever possible. Majer & Svoboda have classified the data according to their quality. When data from this source were not available, the Beilstein database was used. We have not attempted to judge the quality of the latter data according to the criteria of [24]. Instead, we consider that a value of 2.0 kJ/mol is a conservative value that covers the combined uncertainties on these values.

Standard internal energy of vaporization or cohesive energy

The standard internal energy of vaporization or cohesive energy is noted $\Delta_{vap}U°$ and its formal definition is given by eqn 10a:

$$\Delta_{vap}U° = U° - U_{sat}^1 \tag{10a}$$

That is $\Delta_{vap}U°$ is the difference between the energy of the ideal gas at a standard pressure and that of the saturated liquid at this temperature [24] and pressure. Equation 10b follows from this definition:

$$\Delta_{vap}U° = \Delta_{vap}H° - RT \tag{10b}$$

$\Delta_{vap}U°$ has a fundamental physical meaning as it measures the energy necessary to bring the entities (molecules or atoms) of the liquid from their equilibrium distances to an infinite distance.

Fundamental reference texts on the experimental determination and general study of $\Delta_{vap}U°$ are Majer & Svoboda's compilation [24] as well as Barton's *Handbook of Solubility Parameters and Other Cohesion Parameters* [11].

$\Delta_{vap}U°$ values are obtained from the corresponding enthalpies $\Delta_{vap}H°$ through eqn (10b). The latter, in turn, are determined from $\Delta_{vap}H$. It follows that numerical uncertainties on cohesion energies are the

same as for the standard enthalpy of vaporization at 298.15 K. $\Delta_{vap}U°$ is obtained immediately from $\Delta_{vap}H°$.

Cohesive energy density

The quantity $\Delta_{vap}U°/V_m$ plays a key role in the theory of regular solutions [9–11]. It measures the cohesive energy per unit of volume and is termed 'cohesive energy density'. Following Hildebrand, [9–11] its square root $(\Delta_{vap}U°/V_m)^{\frac{1}{2}}$ is represented by δ. Here, the notation δ_H (for 'Hildebrand's delta') is used in order to avoid possible confusions. δ_H is generally known as the 'solubility parameter'. Barton's monograph [11] is a leading reference on the subject.

The values presented here were calculated using the appropriate $\Delta_{vap}U°$ and V_m data also given in this compilation.

The ratio $\Delta_{vap}U°/V_m$ has the dimensions of a pressure. Thus, δ_H has the dimensions of (pressure)$^{\frac{1}{2}}$ and the formal SI unit is Pa$^{\frac{1}{2}}$. On account of the order of magnitude of the δ_H values, MPa$^{\frac{1}{2}}$ units are more convenient [11] and shall be used here.

(A comment on notations: pages 650–651 of the text, and eqns 7–10 closely follow [24]. The notations, however, are different. This is so because they have been adapted to the more recent norms of [18]).

Table 1a

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
gas			1.000	1.00	0.00	0.000	0.000	0.00
Perfluorinated Solvents								
nonaromatic								
1	perfluoro-n-hexane	[355-42-0]	1.252	1.57		0.221	0.222	0.00
2	perfluoro-n-heptane	[355-57-9]	1.261[h]	1.76[h]		0.228	0.275	0.05
3	perfluoro-n-octane	[307-34-6]	1.284[h]	1.81[h]	0.00	0.245	0.288	0.04
4	perfluoro(methylcyclohexane)	[355-02-2]	1.282	1.86	0.28	0.244	0.301	0.06
5	perfluorodecalin; perfluorodecahydronaphthalene	[306-94-5]	1.315 (18 °C)[h]	1.86[h]	0.00	0.267	0.301	0.03
6	perfluoro(1-methyldecalin); perfluoro(1-methyldecahydronaphthalene)	[51294-16-7]	1.317[i]			0.268		
7	perfluorodimethyldecalin	[54471-59-9]						
8	perfluorotri-n-butylamine; heptacosafluorotributylamine	[311-89-7]	1.291 (25 °C)[j]	1.9[j]		0.250	0.310	0.06
aromatic								
9	hexafluorobenzene; perfluorobenzene	[392-56-3]	1.377	2.05	0.00	0.309	0.344	0.04
Cyclic and Acyclic Nonaromatic Hydrocarbons and Related Compounds								
10	2-methylbutane; isopentane	[78-78-4]	1.354[j]	1.828[j]	0.12	0.294	0.293	0.00
11	n-pentane	[109-66-0]	1.358[j]	1.841[j]	0.00	0.296	0.296	0.00
12	n-hexane	[110-54-3]	1.375[j]	1.886[j]	0.00	0.308	0.307	0.00
13	n-heptane	[142-82-5]	1.388	1.94	0.00	0.317	0.320	0.00
14	n-octane	[111-65-9]	1.397[j]	1.948[j]	0.00	0.322	0.322	0.00
15	2,2,4-trimethylpentane; isooctane; isobutyltrimethylmethane	[540-84-1]	1.391[j]	1.94[j]	0.0[j,l]	0.319	0.320	0.00
16	n-nonane	[111-84-2]	1.405[j]	1.970[j]	0.07[l]	0.328	0.327	0.00
17	n-decane	[124-18-5]	1.412[j]	1.989[j]	0.07[l]	0.332	0.331	0.00
18	n-undecane	[1120-21-4]	1.417[h]	2.01[h]		0.335	0.342	0.01
19	n-dodecane	[112-40-3]	1.422[j]	2.002 (30 °C)[j]	0.07[l]	0.338	0.334	0.00
20	n-pentadecane	[629-62-9]	1.432[h]	2.05[h]		0.344	0.344	0.00
21	n-hexadecane	[544-76-3]	1.435[h]	2.05[h]	0.06[l]	0.346	0.344	0.00
22	cyclopentane; pentamethylene	[287-92-7]	1.406[j]	1.969[j]	0.00[m]	0.328	0.326	0.00

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
23	cyclohexane; hexahydrobenzene; hexamethylene	[110-82-7]	1.426[j]	2.024[j]	0.00[l]	0.341	0.339	0.00
24	cycloheptane	[291-64-5]	1.445[h]	2.08[h]		0.352	0.351	0.00
25	cyclooctane	[292-64-8]	1.459[h]	2.12[h]	0.00[m]	0.361	0.359	0.00
26	methylcyclohexane; hexahydrotoluene; cyclohexylmethane	[108-87-2]	1.423[j]	2.020[j]	0.00	0.339	0.338	0.00
27	1-hexene	[592-41-6]	1.388[j]	2.051[j]	0.46[n]	0.317	0.344	0.03
28	cyclohexene; tetrahydrobenzene	[110-83-8]	1.447[j]	2.220[j]	0.33	0.354	0.379	0.03
29	1,4-cyclohexadiene	[628-41-1]	1.473	2.26	0.13[o]	0.369	0.387	0.02
30	cycloheptatriene; cyclohepta-1,3,5-triene	[544-25-2]	1.517	2.54	0.25	0.394	0.435	0.04
31	1,5-cyclooctadiene	[111-78-4]	1.493	2.38	0.17[m]	0.381	0.408	0.03
32	cyclooctatetraene; 1,3,5,7-cyclooctatetraene	[629-20-9]	1.538	2.46	0.07	0.406	0.422	0.02
33	trans,trans,cis,-1,5,9-cyclododecatriene	[2765-29-9]	1.507	2.41	0.35[h,m]	0.389	0.413	0.02
34	dicyclopentadiene; 3a,4,7,7a-tetrahydro-1H-4,7-methano-indene	[77-73-6]	1.511	2.49	0.40[h,m]	0.391	0.427	0.04
35	cis-decalin; cis-decahydronaphthalene; cis-bicyclo[4.4.0]decane	[493-01-6]	1.481	2.23	0.00[m]	0.374	0.381	0.01
36	perhydrofluorene; dodecahydrofluorene	[5744-03-6]	1.502	2.31		0.386	0.396	0.01
37	quadricyclane; quadricyclo[2.2.1.0^{2,6}.0^{3,5}]heptane	[278-06-8]	1.485	2.29		0.376	0.392	0.02
38	tetramethylsilane	[75-76-3]	1.359[j]	1.92[j]	0.48[n]	0.297	0.315	0.02
Aromatic Hydrocarbons								
39	benzene	[71-43-2]	1.501[j]	2.274 (25 °C)[j]	0.00	0.385	0.389	0.00
40	toluene; methyl benzene	[108-88-3]	1.497	2.43	0.38	0.383	0.417	0.03
41	o-xylene; 1,2-dimethylbenzene	[95-47-6]	1.505[j]	2.568[j]	0.63	0.387	0.439	0.05
42	m-xylene; 1,3-dimethylbenzene	[108-38-3]	1.497[j]	2.374[j]	0.31[k]	0.383	0.407	0.02
43	p-xylene; 1,4-dimethylbenzene	[106-42-3]	1.496[j]	2.270[j]	0.00[m]	0.382	0.388	0.01
44	mesitylene; 1,3,5-trimethylbenzene	[108-67-8]	1.499[j]	2.273 (25 °C)[j]	0.10[n]	0.384	0.389	0.01
45	prehnitene; 1,2,3,4-tetramethylbenzene	[488-23-3]	1.515	2.59		0.393	0.443	0.05
46	ethylbenzene; phenylethane	[100-41-4]	1.496[j]	2.404[j]	0.58	0.382	0.412	0.03
47	cumene; isopropyl benzene; 2-phenylpropane; 1-methylethylbenzene	[98-82-8]	1.491[j]	2.383[j]	0.65	0.379	0.409	0.03
48	cyclohexylbenzene; phenylcyclohexane	[827-52-1]	1.526[j]		0.60[k]	0.399		
49	diphenylmethane; 1,1′-methylenebis-benzene; methyl-1,1′-biphenyl	[101-81-5]	1.575	2.61	0.26?[m]	0.425	0.446	0.02
50	1-methylnaphthalene	[90-12-0]	1.618[j]	2.915[j]	0.37[k,n]	0.447	0.489	0.04
51	tetralin; 1,2,3,4-tetrahydronaphthalene	[119-64-2]	1.541[j]	2.773[j]	0.61[k]	0.407	0.470	0.06
Halogenated Compounds								
nonaromatic								
52	carbon tetrachloride; tetrachloromethane	[56-23-5]	1.460	2.30	0.00	0.361	0.394	0.03
53	fluorotrichloromethane; trichlorofluoromethane	[75-69-4]	1.383	2.38	0.48	0.313	0.408	0.10
54	bromotrichloromethane	[75-62-7]	1.506	2.47	0.40[h,n]	0.388	0.424	0.04

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
55	1,1-dichloroethane; ethylidene chloride	[75-34-3]	1.416[j]	10.0 (18 °C)[j]	2.35	0.334	0.818	0.48
56	1,2-dichloroethane; ethylene chloride	[107-06-2]	1.445	10.74	1.36	0.352	0.830	0.48
57	1,1,1-trichloroethane; methyl chloroform	[71-55-6]	1.438	7.33	1.90	0.348	0.760	0.41
58	1,1,2-trichloroethane	[79-00-5]	1.471	7.28	1.36	0.368	0.758	0.39
59	1,1,1-trichlorotrifluoroethane	[354-58-5]	1.360	2.44	0.74[h]	0.298	0.419	0.12
60	1,1,2-trichloro-1,2,2-trifluoroethane	[76-13-1]	1.358[j]	2.41 (25 °C)[j]	0.86[h]	0.297	0.413	0.12
61	1,1-dichloroethylene; 1,1-dichloroethene	[75-35-4]	1.425[j]		1.25[m]	0.340		
62	cis-1,2-dichloroethylene; cis-1,2-dichloroethene	[156-59-2]	1.449[j]	9.20 (25 °C)[j]	2.95	0.355	0.804	0.45
63	trans-1,2-dichloroethylene; trans-1,2-dichloroethene	[156-60-5]	1.446	2.27	0.00[m]	0.353	0.388	0.04
64	trichloroethylene; trichloroethene	[79-01-6]	1.477[j]	3.42 (16 °C)[j]	0.90[o]	0.371	0.548	0.18
65	tetrachloroethylene; tetrachloroethene; ethylene tetrachloride	[127-18-4]	1.505	2.34	0.00[m]	0.387	0.401	0.01
66	1-chloropropane; n-propyl chloride	[540-54-5]	1.388	8.53	2.06	0.317	0.790	0.47
67	1,3-dichloropropane; trimethylene chloride	[142-28-9]	1.448[h]	9.51[h]	2.09	0.354	0.810	0.46
68	2,2-dichloropropane; isopropylidene chloride	[594-20-7]	1.414	11.63	2.35	0.333	0.842	0.51
69	3-chloro-1,1,1-trifluoropropane	[460-35-5]	1.337[h]		1.59[k]	0.283		
70	1,2-dichloro-1,1,2,3,3,3-hexafluoropropane	[661-97-2]	1.303	2.38		0.259	0.408	0.15
71	1,2,3-trichloropropane; glycerin trichlorohydrin	[96-18-4]	1.484	7.90	1.67[m]	0.375	0.775	0.40
72	hexachloropropene	[1888-71-7]	1.550	2.78	0.45[m]	0.412	0.471	0.06
73	1-chlorobutane; n-butyl chloride	[109-69-3]	1.401	7.34	2.11	0.325	0.760	0.44
74	1,4-dichlorobutane; tetramethylen chloride	[110-56-5]	1.454	9.65	2.22	0.358	0.812	0.45
75	hexachloro-1,3-butadiene	[87-68-3]	1.556	2.59	0.2[n]	0.415	0.443	0.03
76	1,2-dichloro-1,2,3,3,4,4-hexafluorocyclobutane	[356-18-3]	1.333	2.46		0.280	0.422	0.14
77	hexachlorocyclopentadiene	[77-47-4]	1.564[p]	2.91[p]	0.88[q]	0.420	0.489	0.07
78	chlorocyclohexane; cyclohexyl chloride	[542-18-7]	1.463[h]	7.60[h]	2.19[m]	0.363	0.767	0.40
79	1,10-dichlorodecane; decamethylen chloride	[2162-98-3]	1.460	7.07	2.62[q]	0.361	0.752	0.39
80	methyltrichlorosilane; trichloromethylsilane	[75-79-6]	1.412[h]		1.89	0.332		
81	bromoethane; ethyl bromide	[74-96-4]	1.424	9.59	2.04	0.339	0.811	0.47
82	1,2-dibromoethane; ethylene bromide	[106-93-4]	1.539[j]	4.750 (30 °C)[j]	1.04	0.406	0.652	0.25
83	1-bromopropane; n-propyl bromide	[106-94-5]	1.433	8.44	2.12	0.345	0.788	0.44
84	1-bromobutane; n-butyl bromide	[109-65-9]	1.439	7.16	2.14	0.349	0.755	0.41
85	iodomethane; methyl iodide	[74-88-4]	1.530	6.92	1.63	0.401	0.747	0.35
86	diiodomethane; methylene iodide	[75-11-6]	1.741[j]	5.316 (25 °C)[j]	1.15[k]	0.504	0.683	0.18
87	iodoethane; ethyl iodide	[75-03-6]	1.513	7.77	1.80	0.392	0.772	0.38
88	1-iodopropane; n-propyl iodide	[107-08-4]	1.505	7.09	2.01	0.387	0.753	0.37
89	2-iodopropane; isopropyl iodide	[75-30-9]	1.499[j]	8.19[j]	2.09[m]	0.384	0.782	0.40
90	1-iodobutane; n-butyl iodide	[542-69-8]	1.499	6.35	2.10	0.384	0.728	0.34
aromatic								
91	fluorobenzene; phenyl fluoride	[462-06-6]	1.465	5.55	1.61	0.364	0.695	0.33

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
92	1,2-difluorobenzene	[367-11-3]	1.443	14.26	2.53	0.351	0.869	0.52
93	1,3-difluorobenzene	[372-18-9]	1.437	5.24	1.55	0.347	0.679	0.33
94	1,4-difluorobenzene	[540-36-3]	1.441	2.26	0.00[k]	0.350	0.387	0.04
95	1,3,5-trifluorobenzene	[372-38-3]	1.414		0.00[k]	0.333		
96	(trifluoromethyl)benzene; α,α,α-trifluorotoluene	[98-08-8]	1.415[h]	9.40[h]	2.86	0.334	0.808	0.47
97	2,3,4,5,6-pentafluorotoluene	[771-56-2]	1.402	1.93	2.01[k]	0.326	0.317	0.01
98	chlorobenzene; phenyl chloride	[108-90-7]	1.524	5.74	1.72	0.398	0.703	0.31
99	1,2-dichlorobenzene	[95-50-1]	1.551	10.36	2.53	0.413	0.824	0.41
100	1,3-dichlorobenzene	[541-73-1]	1.546	5.16	1.68	0.410	0.675	0.27
101	1,4-dichlorobenzene	[106-46-7]	1.528 (60 °C)[j]	2.41 (50 °C)[j]	0.00	0.400	0.413	0.01
102	1,2,3-trichlorobenzene	[87-61-6]	1.550[h]		2.39[n]	0.412		
103	1,2,4-trichlorobenzene	[120-82-1]	1.571	4.15	1.26[n]	0.423	0.612	0.19
104	1,2,3,4-tetrachlorobenzene	[634-66-2]	1.58[r]	3.2[h]	1.90[n]	0.428	0.524	0.10
105	1-chloronaphthalene; 1-naphthyl chloride	[90-13-1]	1.633[h]	5.0[h]	1.55[n]	0.455	0.667	0.21
106	bromobenzene; phenyl bromide	[108-86-1]	1.560	5.55	1.74	0.418	0.695	0.28
107	1,2-dibromobenzene	[583-53-9]	1.611	8.07	2.06[n]	0.444	0.779	0.34
108	1,3-dibromobenzene	[108-36-1]	1.607	5.00	1.37[n]	0.442	0.667	0.23
109	2,5-dibromotoluene	[615-59-8]	1.602			0.439		
110	iodobenzene; phenyl iodide	[591-50-4]	1.620	4.75	1.71	0.488	0.652	0.20
111	1-iodonaphthalene; 1-naphthyl iodide	[90-14-2]	1.702	4.56	1.44[n]	0.487	0.640	0.15
Nitriles								
112	acetonitrile; ethanenitrile; methyl cyanide; cyanomethane	[75-05-8]	1.344[j]	35.94 (25 °C)[j]	3.95	0.287	0.946	0.66
113	propionitrile; propanenitrile; ethyl cyanide	[107-12-0]	1.366	28.86[j]	4.04	0.302	0.933	0.63
114	butyronitrile; butanenitrile; n-propyl cyanide; 1-cyanopropane	[109-74-0]	1.383	24.56	4.07	0.313	0.922	0.61
115	valeronitrile; pentanenitrile; n-butyl cyanide	[110-59-8]	1.397	20.03	4.12	0.322	0.905	0.58
116	hexanenitrile; capronitrile; n-amyl cyanide; n-pentyl cyanide	[628-73-9]	1.407[j]	17.26 (25 °C)[j]	3.48[h,l]	0.329	0.890	0.56
117	undecanenitrile; decyl cyanide	[2244-07-7]	1.433	10.86	3.38[h,l]	0.345	0.831	0.49
118	dodecanenitrile; undecyl cyanide; lauronitrile	[2437-25-4]	1.435	10.11	3.36[h,l]	0.346	0.820	0.47
119	chloroacetonitrile; chloroethanenitrile	[107-14-2]	1.422	30.0[h]	3.00[q]	0.338	0.935	0.60
120	trichloroacetonitrile; trichloroethanenitrile	[545-06-2]	1.440	7.74	2.0[q]	0.349	0.771	0.42
121	pivalonitrile; 2,2-dimethylpropanenitrile; tert-butyl cyanide; trimethylacetonitrile	[630-18-2]	1.377	20.09	4.15	0.309	0.905	0.60
122	3-methoxypropanenitrile	[110-67-8]	1.403[h]		3.47	0.326		
123	acrylonitrile; 2-propenenitrile; vinyl cyanide; cyanoethylene	[107-13-1]	1.391[j]	33.01[j]	3.90	0.319	0.941	0.62
124	benzonitrile; phenyl cyanide; cyanobenzene	[100-47-0]	1.528[j]	25.20 (25 °C)[j]	4.28	0.400	0.924	0.52
125	phenylacetonitrile; benzyl cyanide; benzeneacetonitrile	[140-29-4]	1.522	19.50	3.59[o]	0.397	0.902	0.51
126	N,N-dimethylcyanamide; dimethyl-carbamonitrile	[1467-79-4]	1.409	37.23	4.77	0.330	0.948	0.62
127	N,N-diethylcyanamide; diethyl-carbamonitrile	[617-83-4]	1.424[h]			0.339		
128	N,N-diisopropylcyanamide; diisopropyl-carbamonitrile	[3085-76-5]	1.427[h]		4.80[q]	0.341		

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
Ethers and Orthoesters								
129	diethyl ether; ethyl ether; ethoxyethane; 1,1′-oxybisethane	[60-29-7]	1.352	4.42	1.11	0.293	0.631	0.34
130	di-n-propyl ether; n-propyl ether; 1,1′-oxybispropane	[111-43-3]	1.381[j]	3.39 (26 °C)[j]	1.12	0.312	0.544	0.23
131	diisopropyl ether; isopropyl ether; 2,2′-oxybispropane	[108-20-3]	1.367	4.04	1.13	0.303	0.603	0.30
132	di-n-butyl ether; n-butyl ether	[142-96-1]	1.398	3.18	1.18	0.323	0.522	0.20
133	di-tert-butyl ether; tert-butyl ether	[6163-66-2]	1.394	3.05	1.25[n]	0.321	0.506	0.19
134	diphenyl ether; phenyl ether; 1,1′-oxybisbenzene; diphenyl oxide; phenoxybenzene	[101-84-8]	1.581[j]	3.686[j]	1.17	0.429	0.573	0.14
135	dibenzyl ether; benzyl ether; 1,1′-[oxybis(methylene)]bisbenzene	[103-50-4]	1.562	3.86	1.39[n]	0.419	0.588	0.17
136	n-butyl methyl ether; 1-methoxybutane	[628-28-4]	1.374[h]		1.27[k]	0.307		
137	tert-butyl methyl ether; 2-methoxy-2-methylpropane	[1634-04-4]	1.369[h]		1.36[n]	0.304		
138	tert-butyl ethyl ether; 2-ethoxy-2-methylpropane	[637-92-3]	1.376[h]		1.22[n]	0.309		
139	tert-amyl methyl ether; 2-methoxy-2-methylbutane	[994-05-78]	1.388[h]			0.317		
140	ethyl vinyl ether; ethoxyethene	[109-92-2]	1.375[j]		0.98	0.308		
141	anisole; methyl phenyl ether; methoxybenzene	[100-66-3]	1.517	4.45	1.36	0.394	0.633	0.24
142	phenetole; ethyl phenyl ether; ethoxybenzene	[103-73-1]	1.507[j]	4.22[j]	1.41	0.389	0.617	0.23
143	cineole; 1,3,3-trimethyl-2-oxabicyclo[2,2,2]octane	[470-82-6]	1.458	4.84	1.58	0.360	0.658	0.30
144	bis(2-chloroethyl) ether; 1,1′-oxybis[2-chloroethane]; 2,2′-dichlorodiethyl ether	[111-44-4]	1.457	20.79	2.43[q]	0.360	0.908	0.55
145	dimethoxymethane; methylal	[109-87-5]	1.354[j]	2.645[j]	0.91	0.294	0.451	0.16
146	diethoxymethane	[462-95-3]	1.373[h]	2.53[h]	1.25	0.307	0.433	0.13
147	ethylene glycol dimethyl ether; 1,2-dimethoxyethane;monoglyme	[110-71-4]	1.380[j]	7.20 (25 °C)[j]	1.61[q]	0.311	0.756	0.45
148	diethylene glycol dimethyl ether; bis(2-methoxyethyl) ether; diglyme; 1,1′-oxybis[2-methoxyethane]	[111-96-6]	1.408[j]	7.3[j]	1.92[q]	0.329	0.759	0.43
149	triethylene glycol dimethyl ether; triglyme	[112-49-2]	1.423[h]	7.5 (25 °C)[h]	2.16[q]	0.339	0.765	0.43
150	diethylene glycol diethyl ether; bis(2-ethoxyethyl) ether; 1,1′-oxybis(2-ethoxyethane)	[112-36-7]	1.411[j]	5.70 (25 °C)[j]	1.96[n]	0.331	0.701	0.37
151	1,2-dimethoxybenzene; veratrole	[91-16-7]	1.532 (25 °C)[j]	4.09 (25 °C)[j]	1.35[m]	0.402	0.607	0.21
152	trimethyl orthoformate; trimethoxymethane	[149-73-5]	1.379[h]		1.70[q]	0.311		
153	trimethyl orthoacetate; 1,1,1-trimethoxyethane	[1445-45-0]	1.388[h]		1.48[n]	0.317		
154	furan; oxole; furfuran	[110-00-9]	1.421[j]	2.942 (25 °C)[j]	0.69	0.338	0.493	0.16
155	tetrahydrofuran; oxolane; oxacyclopentane; diethylene oxide; tetramethylene oxide	[109-99-9]	1.406	7.47	1.69	0.328	0.764	0.44
156	2-methyltetrahydrofuran; 1,4-oxidopentane	[96-47-9]	1.408[j]	6.97 (25 °C)[j]	1.38[h]	0.329	0.749	0.42
157	2,5-dimethyltetrahydrofuran (cis + trans)	[1003-38-9]	1.394	3.05		0.321	0.506	0.19

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
158	2,2,5,5-tetramethyltetrahydrofuran	[15045-43-9]	1.404	5.03		0.325	0.668	0.34
159	tetrahydropyran; oxane; pentamethylene oxide; oxacyclohexane	[142-68-7]	1.420	5.68	1.74	0.337	0.701	0.36
160	(±)-3-methyltetrahydropyran	[26093-63-0]	1.421[h]			0.338		
161	1,4-dioxane; p-dioxane; diethylene dioxide	[123-91-1]	1.422	2.27	0.46	0.338	0.388	0.05
162	1,3-dioxolane; ethylene glycol methylene ether	[646-06-0]	1.404		1.19	0.327		
163	5-acetyl-5-methyl-1,3-dioxane	[3495-19-0]	1.455[h]			0.358		
164	2-methoxy-1,3-dioxolane	[19693-75-5]	1.410[h]		1.87[m]	0.331		
165	(±)-methyloxirane; propylene oxide	[75-56-9]	1.366[j]		2.00[k]	0.302		
166	(±)-chloromethyl)oxirane; epichlorohydrin; 1-chloro-2,3-epoxypropane	[106-89-8]	1.438[j]	22.6 (22 °C)[j]	2.02′	0.348	0.915	0.57

Acyl Compounds

ketones

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
167	acetone; 2-propanone; dimethyl ketone	[67-41-1]	1.359	21.36	2.88	0.298	0.911	0.61
168	2-butanone; methyl ethyl ketone	[78-93-3]	1.379	18.85	2.78	0.311	0.899	0.59
169	3-methyl-2-butanone; isopropyl methyl ketone	[563-80-4]	1.388[h]	16.57[h]	2.79[n]	0.317	0.886	0.57
170	3,3-dimethyl-2-butanone; tert-butyl methyl ketone; pinacolone	[75-97-8]	1.397[h]	12.73[h]	2.75[n]	0.322	0.854	0.53
171	2-pentanone; n-propyl methyl ketone	[107-87-9]	1.391[j]	15.38[j]	2.74[n]	0.318	0.878	0.56
172	3-pentanone; diethyl ketone	[96-22-0]	1.391	17.45	2.70[q]	0.319	0.892	0.57
173	4-methyl-2-pentanone; isobutyl methyl ketone	[108-10-1]	1.396[j]	13.11[j]	2.69[n]	0.322	0.858	0.54
174	2,4-dimethyl-3-pentanone; diisopropyl ketone	[565-80-0]	1.399	17.07	2.76[q]	0.324	0.889	0.57
175	2,2,4,4-tetramethyl-3-pentanone; di-tert-butyl ketone	[815-24-7]	1.419	9.36	2.51[k]	0.336	0.807	0.47
176	2~hexanone; methyl n-butyl ketone	[591-78-6]	1.401[j]	14.56[j]	2.69[o]	0.325	0.871	0.55
177	4-heptanone; di-n-propyl ketone	[123-19-3]	1.407[h]	12.6[h]	2.68[q]	0.329	0.853	0.52
178	2,6-dimethyl-4-heptanone; diisobutyl ketone; isovalerone	[108-83-8]	1.412[j]	9.91[h]	2.66[m]	0.333	0.817	0.48
179	5~nonanone; di-n-butyl ketone	[502-56-7]	1.420[h]	10.6[h]	2.71[q]	0.337	0.828	0.49
180	cyclopentanone	[120-92-3]	1.437	14.45	3.28	0.347	0.871	0.52
181	cyclohexanone; cyclohexyl ketone	[108-94-1]	1.451	16.02	3.06	0.356	0.882	0.53
182	cyclopropyl methyl ketone; cyclopropylmethylmethanone	[765-43-5]	1.425[h]		2.73	0.340		
183	dicyclopropyl ketone; dicyclopropylmethanone	[1121-37-5]	1.467[h]		2.83[k]	0.365		
184	acetophenone; acetylbenzene; 1-phenylethanone; methyl phenyl ketone	[98-86-2]	1.534	18.18	3.05	0.404	0.896	0.49
185	2,4-pentanedione; acetylacetone	[123-54-6]	1.451[j]	25.7[j]	3.03	0.356	0.925	0.57
186	1,1,1-trichloroacetone	[918-00-3]	1.462	10.37		0.362	0.824	0.46
187	hexachloroacetone	[116-16-5]	1.511	3.99	1.24[m]	0.391	0.599	0.21
188	1,1,1-trichloro-3,3,3-trifluoroacetone	[758-42-9]	1.382 (25 °C)[h]			0.313		

esters, lactones, anhydrides

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
189	methyl formate; methyl methanoate	[107-31-3]	1.343	8.73	1.77	0.287	0.794	0.51
190	methyl acetate; methyl ethanoate	[79-20-9]	1.361	6.94	1.69	0.299	0.748	0.45
191	methyl propionate; methyl propanoate	[554-12-1]	1.376	6.23	1.67	0.309	0.723	0.41

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
192	methyl butyrate; methyl butanoate	[623-42-7]	1.386	5.50	1.72[n]	0.317	0.692	0.38
193	methyl valerate; methyl pentanoate	[624-24-8]	1.397	5.02	1.62[n]	0.322	0.668	0.35
194	methyl caproate; methyl hexanoate	[106-70-7]	1.404	4.70	1.70[q]	0.328	0.649	0.32
195	methyl caprylate; methyl octanoate	[111-11-5]	1.417	4.13	1.67[q]	0.335	0.610	0.28
196	methyl caprate; methyl decanoate	[110-42-9]	1.425	3.86	1.65[q]	0.341	0.588	0.25
197	methyl laurate; methyl dodecanoate	[111-82-0]	1.431	3.60	1.70[q]	0.344	0.565	0.22
198	methyl oleate; methyl (Z)-9-octadecenoate	[112-62-9]	1.451	3.24	1.60[k]	0.356	0.528	0.17
199	methyl linoleate	[112-63-0]	1.461	3.20		0.362	0.524	0.16
200	methyl acrylate; methyl 2-propenoate	[96-33-3]	1.408[j]	7.12[h]	1.75[n]	0.329	0.754	0.43
201	methyl methacrylate; methyl 2-methyl-2-propenoate	[80-62-6]	1.415[j]	2.9[j]	1.76[n]	0.334	0.487	0.15
202	methyl benzoate; methyl benzenecarboxylate	[93-58-3]	1.517[j]	6.59[j]	1.92[k]	0.394	0.736	0.34
203	methyl trifluoroacetate; methyl trifluoroethanoate	[431-47-0]	1.291	11.46	2.48[o]	0.260	0.839	0.58
204	methyl trichloroacetate	[598-99-2]	1.457	8.79	2.33[o]	0.360	0.796	0.44
205	ethyl formate; ethyl methanoate	[109-94-4]	1.360[j]	7.16 (25 °C)[j]	1.94	0.298	0.755	0.46
206	ethyl acetate; ethyl ethanoate	[141-78-6]	1.372	6.03	1.78	0.306	0.716	0.41
207	ethyl acetoacetate; ethyl acetoethanoate; ethyl 3-oxobutanoate	[141-97-9]	1.421[j]	15.7 (22 °C)[j]	2.96	0.338	0.880	0.54
208	ethyl lactate; ethyl 2-hydroxypropionate	[97-64-3]	1.412[j]	13.1[j]	2.55[k]	0.332	0.858	0.53
209	ethyl benzoate; ethyl benzenecarboxylate	[93-89-0]	1.505	6.13	1.95	0.387	0.719	0.33
210	ethyl chloroacetate; ethyl chloroethanoate	[105-39-5]	1.421	12.78	2.65[n]	0.338	0.855	0.52
211	ethyl trichloroacetate; ethyl trichloroethanoate	[515-84-4]	1.450	9.03	2.60[q]	0.355	0.801	0.45
212	n-propyl formate; n-propyl methanoate	[110-74-7]	1.377[j]	7.72 (19 °C)[j]	1.83[n]	0.309	0.771	0.46
213	n-propyl acetate; n-propyl ethanoate	[109-60-4]	1.384[j]	6.002[j]	1.79[o]	0.314	0.714	0.40
214	n-butyl acetate; n-butyl ethanoate	[123-86-4]	1.394[j]	5.01[j]	1.86[n]	0.320	0.667	0.35
215	isoamyl acetate; isopentyl acetate; 3-methyl-1-butyl acetate	[123-92-2]	1.401[j]	4.63 (30 °C)[j]	1.84[n]	0.325	0.645	0.32
216	vinyl acetate; vinyl ethanoate; ethenyl acetate	[108-05-4]	1.396[j]	2.3[h]	1.61[m]	0.321	0.394	0.07
217	dimethyl carbonate; methyl carbonate	[616-38-6]	1.368	3.17	0.93	0.304	0.520	0.22
218	diethyl carbonate; ethyl carbonate	[105-58-8]	1.385	2.88	1.07	0.315	0.485	0.17
219	diethyl malonate; ethyl malonate; diethyl propanedioate	[105-53-3]	1.414[j]	7.87 (25 °C)[j]	2.57[m]	0.333	0.775	0.44
220	1,3-dioxolan-2-one; ethylene carbonate; cyclic ethylene carbonate	[96-49-1]	1.420 (40 °C)[j]	89.78 (40 °C)[j]	4.51	0.337	0.978	0.64
221	4,5-dichloro-1,3-dioxolan-2-one	[3967-55-3]	1.463	34.36	3.47[n]	0.363	0.943	0.58
222	(±)-propylene carbonate; 4-methyl-1,3-dioxolan-2-one	[108-32-7]	1.421	62.93	4.77[n]	0.338	0.969	0.63
223	γ-butyrolactone; 2(3H)-dihydrofuranone; 4-hydroxybutyric acid γ-lactone	[96-48-0]	1.437	40.96	4.27	0.347	0.952	0.61
224	γ-valerolactone; tetrahydropyran-2-one	[542-28-9]	1.457	36.14	4.71[h]	0.358	0.946	0.59
225	acetic anhydride; acetic acid anhydride; ethanoic anhydride	[108-24-7]	1.390[j]	20.7 (19 °C)	2.8	0.318	0.908	0.59

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
226	trichloroacetic anhydride	[4124-31-6]	1.484	5.00[h]		0.375	0.667	0.29
227	triacetin; glyceryl triacetate; 1,2,3-propanetriol triacetate	[102-76-1]	1.428	7.01	2.73[n]	0.344	0.750	0.41
228	triolein; 1,2,3-propanetriyl-tri-(Z)-9-octadecenoate; glycerol trioleate	[122-32-7]	1.468	3 .8[h]	3.12[n]	0.366	0.583	0.22
229	dimethyl phthalate	[131-11-3]	1.516[h]	8.66[h]	2.66[n]	0.394		
230	di-n-butyl phthalate	[84-74-2]	1.493[j]	6.44 (30 °C)[j]	2.83[n]	0.381	0.731	0.35
Di-substituted Amides and Thioamides and Tetrasubstituted Ureas								
231	N,N-dimethylformamide (DMF)	[68-12-2]	1.430	37.06	3.79	0.343	0.947	0.60
232	N,N-dimethylacetamide	[127-19-5]	1.438	38.30	3.78	0.348	0.949	0.60
233	N,N-dimethylpropionamide; ethyl-N,N′-dimethyl formamide	[758-96-3]	1.439	33.08	3.78[o]	9.349	0.941	0.59
234	N,N-diethylformamide	[617-84-5]	1.434	29.02	3.93[n]	0.346	0.933	0.59
235	N,N-diethylacetamide	[685-91-6]	1.439	31.33	3.81[k]	0.349	0.938	0.59
236	N,N-dimethylthioformamide; thioformyldimethylamine	[758-16-7]	1.574[h]		4.46[m]	0.425		
237	N-methylformanilide	[93-61-8]	1.561	17.21		0.418	0.890	0.47
238	1,1,3,3-tetramethylurea	[632-22-4]	1.450	24.46	3.47[q]	0.355	0.921	0.57
239	1,1,3,3-tetraethylurea	[1187-03-7]	1.446	14.74	3.28[o]	0.353	0.873	0.52
240	1-formylpiperidine; piperidine-1-carbaldehyde; 1-piperidinecarboxaldehyde	[2591-86-8]	1.484	26.15		0.375	0.926	0.55
241	1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidone; N,N′-dimethyl-N,N′-trimethyleneurea (DMPU)	[7226-23-5]	1.488 (25 °C)[h]	36.12 (25 °C)[h]	4.17[n]	0.378	0.946	0.57
242	1-methyl-2-pyrrolidinone; N-methylpyrrolidone	[872-50-4]	1.469	32.58	3.75[k]	0.367	0.940	0.57
243	1-methylpyrrolidine-2-thione	[10441-57-3]	1.582[h]			0.429		
244	1-ethyl-2-pyrrolidone; 1-ethyl-pyrrolidin-2-one	[2687-91-4]	1.466[h]			0.365		
245	1-cyclohexyl-2-pyrrolidone; 1-cyclohexyl-pyrrolidin-2-one	[6837-24-7]	1.499 (24 °C)[h]			0.384		
246	1-methylhexahydroazepin-2-one; N-methyl-ε-caprolactam; 1-methyl-azepan-2-one	[2556-73-2]	1.483[h]		4.23[n]	0.375		
247	pyrrolidine-1-carbonitrile; N-cyanopyrrolidine	[1530-88-7]	1.467 (23 °C)[h]		4.85[n]	0.365		
248	piperidine-1-carbonitrile; N-cyanopiperidine	[1530-87-6]	1.471 (18 °C)[h]		4.65[n]	0.368		
249	morpholine-4-carbonitrile; N-cyanomorpholine	[1530-89-8]	1.472[h]		3.25[n]	0.368		
Phosphates, HMPA								
250	trimethyl phosphate; phosphoric acid trimethyl ester; methyl phosphate	[512-56-1]	1.396	21.26	2.82[q]	0.322	0.910	0.59
251	triethyl phosphate; phosphoric acid triethyl ester; ethyl phosphate	[78-40-0]	1.405[j]	13.01 (21 °C)[j]	2.86[q]	0.328	0.857	0.53
252	tri-n-propyl phosphate; phosphoric acid tripropyl ester; propyl phosphate	[513-08-6]	1.417[h]	10.93[h]	2.93[q]	0.335	0.832	0.50
253	tri-n-butylphosphate; phosphoric acid tributyl ester; butyl phosphate	[126-73-8]	1.423	8.29	2.92[q]	0.339	0.785	0.45
254	diethylchlorophosphate; phosphorochloridic acid diethyl ester; diethyl phosphorochloridate	[814-49-3]	1.417		3.57[q]	0.335		

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
255	hexamethylphosphorictriamide; hexamethylphosphoramide (HMPA)	[680-31-9]	1.458	29.00	4.19[k]	0.360	0.933	0.57
256	hexamethylphosphorothioic acid triamide (HMPTA)	[3732-82-9]	1.507 (30 °C)[h]		4.83[m]	0.389		
257	methylphosphonic acid bis(dimethylamide)	[2511-17-3]	1.460[h]			0.361		
Sulfates, Sulfites, Sulfoxides, Sulfamides								
258	dimethyl sulfate; sulfuric acid dimethyl ester	[77-78-1]	1.386	50.28	4.02[m]	0.315	0.961	0.65
259	dimethyl sulfite; methyl sulfite; sulfurous acid dimethyl ester	[616-42-2]	1.409	21.89	2.84[m]	0.330	0.913	0.58
260	diethyl sulfite; ethyl sulfite; sulfurous acid diethyl ester	[623-81-4]	1.414	16.20	3.09[k]	0.333	0.884	0.55
261	dimethyl sulfoxide (DMSO); methyl sulfoxide; sulfinylbismethane	[67-68-5]	1.479	46.71	3.96	0.372	0.958	0.59
262	tetramethylene sulfoxide; tetrahydrothiophene-1-oxide	[1600-44-8]	1.521	42.84	4.17[n]	0.396	0.945	0.55
263	sulfolane; tetramethylene sulfone; tetrahydrothiophene 1,1-dioxide	[126-33-0]	1.481	42.13	4.68[m]	0.374	0.954	0.58
264	methyl methylthiomethyl sulfoxide; methylmethylsulfinylmethyl sulfide; methanesulfinyl-methylsulfonyl-methane	[33577-16-1]	1.552[h]			0.413		
265	3-methyltetrahydrothiophene-1,1-dioxide; 3-methylsulfolane	[872-93-5]	1.477[h]	29.40[h]		0.371	0.934	0.56
266	N,N,N′,N′-tetraethylsulfamide	[2832-49-7]	1.448[h]			0.354		
Pyridines								
267	pyridine; azine	[110-86-1]	1.509	13.22	2.21	0.390	0.859	0.47
268	2-picoline; 2-methylpyridine	[109-06-8]	1.501[j]	9.8[j]	1.91	0.385	0.815	0.43
269	4-picoline; 4-methylpyridine	[108-89-4]	1.505	12.28	2.70	0.387	0.849	0.46
270	2,6-lutidine; 2,6-dimethylpyridine	[108-48-5]	1.497[j]	7.33[j]	1.68[k]	0.383	0.760	0.38
271	3,4-lutidine; 3,4-dimethylpyridine	[583-58-4]	1.511	11.47	1.87[l]	0.391	0.840	0.45
272	2,4,6-collidine; 2,4,6-trimethylpyridine	[108-75-8]	1.498	12.02	2.04[k]	0.383	0.845	0.46
273	2,6-di-tert-butylpyridine	[585-48-8]	1.473	3.39	1.32[h,n]	0.369	0.544	0.17
274	2-cyanopyridine; 2-pyridinecarbonitrile	[100-70-9]	1.525 (30 °C)[h]	93.77 (30 °C)[h]	1.96	0.399	0.979	0.58
275	2-fluoropyridine	[372-48-5]	1.467	37.29	3.37	0.365	0.948	0.58
276	2,6-difluoropyridine	[1513-65-1]	1.437	107.80	3.50	0.347	0.982	0.64
277	pentafluoropyridine; perfluoropyridine	[700-16-3]	1.384[h]		0.98	0.314		
278	2-chloropyridine	[109-09-1]	1.532[h]		3.19[k]	0.402		
279	2-bromopyridine	[109-04-6]	1.571	24.02	3.11[n]	0.423	0.920	0.50
280	3-bromopyridine	[626-55-1]	1.571	9.85	1.99[k]	0.423	0.816	0.39
281	pyrimidine	[298-95-2]	1.496[h]		2.33	0.382		
282	quinoline	[91-22-5]	1.627[j]	8.95 (25 °C)[j]	2.25	0.452	0.799	0.35
Tertiary Amines								
283	triethylamine; N,N-diethylethanamine	[121-44-8]	1.401	2.45	0.72	0.325	0.420	0.10
284	tri-n-butylamine; N,N-dibutyl-1-butanamine	[102-82-9]	1.428	2.29	0.76[q]	0.342	0.392	0.05
285	N,N-dimethylcyclohexylamine	[98-94-2]	1.454	2.86	0.76[k]	0.358	0.482	0.12
286	N,N-dimethylbenzylamine	[103-83-3]	1.501[h]		0.63[k]	0.385		
287	N,N-dimethylaniline; N,N-dimethylbenzenamine	[121-69-7]	1.559[j]	4.91[j]	1.61	0.417	0.662	0.25
288	1-methylpiperidine	[626-67-5]	1.437	2.59	0.77[k]	0.347	0.443	0.10
289	1-methylimidazole	[616-47-7]	1.496[h]		3 .80[n]	0.382		

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
290	1,4-dimethylpiperazine	[106-58-1]	1.447[h]		0.52[n]	0.354		
	Sulfides and Disulfides							
291	dimethyl sulfide; methyl sulfide; thiobismethane; 2-thiapropane	[75-18-3]	1.435	6.42	1.50	0.346	0.730	0.38
292	diethyl sulfide; ethyl sulfide; 1,1'-thiobisethane; 3-thiapentane	[352-93-2]	1.442	6.14	1.52	0.350	0.720	0.37
293	diisopropyl sulfide; isopropyl sulfide; 2,2'-thiobispropane	[625-80-9]	1.438	5.81	1.67[n]	0.348	0.706	0.36
294	di-n-butyl sulfide; n-butyl sulfide; 1,1'-thiobisbutane	[544-40-1]	1.452	4.41	1.59[n]	0.356	0.630	0.27
295	di-tert-butyl sulfide; tert-butyl sulfide; 2,2'-thiobis(2-methylpropane)	[107~47-1]	1.455[h]		1.50[n]	0.358		
296	dimethyl disulfide; methyl disulfide	[624-92-0]	1.525	9.77	1.99	0.399	0.814	0.42
297	diethyl disulfide; ethyl disulfide	[110-81-6]	1.507[h]		2.01[n]	0.389		
298	trimethylene sulfide; thiacyclobutane	[287-27-4]	1.509[h]		1.85	0.390		
299	thiophene; thiofuran; thiofurfuran	[110-02-1]	1.529[j]	2.705 (25 °C)[j]	0.56	0.401	0.460	0.06
300	tetrahydrothiophene; thiacyclopentane; diethylene sulfide	[110-01-0]	1.504	8.61	1.89	0.387	0.792	0.41
301	pentamethylene sulfide; tetrahydrothiopyran; thiacyclohexane	[1613-51-0]	1.506	6.58	1.71[k]	0.388	0.736	0.35
302	thioanisole; methylthiobenzene; phenyl methylmethylthiosulfide; phenyl 1-thiaethane	[100-68-5]	1.587	4.76	1.31[m]	0.432	0.653	0.22
	Nitro Compounds							
303	nitromethane	[75-52-5]	1.381	36.16	3.50	0.312	0.946	0.63
304	nitroethane	[79-24-3]	1.391	28.96	3.61	0.319	0.933	0.61
305	2-nitropropane	[79-46-9]	1.394	27.27	3.76	0.320	0.929	0.61
306	2-methyl-2-nitropropane	[594-70-7]	1.397	23.68	3.74	0.322	0.919	0.60
307	nitrocyclohexane	[1122-60-7]	1.462[h]		3.6[k]	0.362		
308	nitrobenzene	[98-95-3]	1.551	36.09	4.23	0.413	0.946	0.53
	Weak Hydrogen-Bonding Donors							
	Primary and secondary amines							
309	n-butylamine; 1-butanamine; 1-aminobutane	[109-73-9]	1.405	4.92	1.00	0.328	0.662	0.33
310	tert-butylamine; 2-methyl-2-propanamine	[74-64~9]	1.379	4.31	1.15[k]	0.311	0.623	0.31
311	allylamine; 2-propen-1-amine; 2-propenylamine; 3-aminopropylene	[107-11-9]	1.421	5.96	1.13-1.36[t]	0.338	0.713	0.38
312	propargylamine; 2-propyn-1-amine	[2450-71-7]	1.448	6.65	0.74	0.354	0.739	0.39
313	diethylamine; N-ethylethanamine	[109-89-7]	1.386	3.92	1.03	0.315	0.593	0.28
314	diisopropylamine; N-(1-methylethyl)-2-propanamine	[108-18-9]	1.392	3.04	1.20[k]	0.319	0.505	0.19
315	diallylamine	[124-02-7]	1.441	3.78	1.20[n]	0.350	0.582	0.23
316	cyclohexylamine; cyclohexanamine; aminocyclohexane; hexahydroaniline	[108-91-8]	1.459	4.43	1.31[q]	0.361	0.632	0.27
317	N-methylcyclohexylamine; N-methylcyclohexanamine	[100-60-7]	1.455	3.64	1.29[n]	0.358	0.569	0.21
318	piperidine; hexahydropyridine; pentamethylenimine	[110-89-4]	1.453[j]	5.8[j]	0.66-0.80[u]	0.357	0.706	0.35
319	morpholine; tetrahydro-2H-1,4-oxazine; diethylene oximide	[110-91-8]	1.454	7.68	1.71	0.358	0.770	0.41
320	pyrrole; azole	[109-97-7]	1.509	8.03	1.71	0.390	0.779	0.39

Table 1a *Continued*

No.	Compounds	CAS reg. number[a]	n[b]	ε_r[c]	μ[d]	$f(n)$[e]	$g(\varepsilon_r)$[f]	$[g(\varepsilon_r) - f(n)]$[g]
321	1-methylpyrrole	[96-54-8]	1.488[h]		2.12	0.378		
322	N-benzylmethylamine	[103-67-3]	1.522	4.08		0.397	0.606	0.21
323	N-(tert-butyl)benzylamine	[3378-72-1]	1.497	3.24		0.383	0.528	0.15
324	aniline; aminobenzene; phenylamine	[62-53-3]	1.585	7.16	1.51	0.431	0.755	0.32
325	N-methylaniline; N-methylbenzenamine	[100-61-8]	1.571[j]	5.90[h]	1.73[q]	0.423	0.710	0.29
CH acids								
326	dichloromethane; methylene chloride	[75-09-2]	1.424	9.02	1.60	0.339	0.800	0.46
327	chloroform; trichloromethane	[67-66-3]	1.446	4.89	1.02	0.353	0.660	0.31
328	dibromomethane; methylene bromide	[74-95-3]	1.542[h]	7.41[h]	1.78	0.408	0.762	0.35
329	bromoform; tribromomethane	[75-25-2]	1.598[j]	4.39[j]	1.00	0.437	0.629	0.19
330	1,1,2,2-tetrachloroethane; acetylene tetrachloride	[79-34-5]	1.494	8.42	1.33	0.381	0.788	0.41
331	pentachloroethane	[76-01-7]	1.503	3.90	0.92	0.386	0.592	0.21
332	propargyl chloride; 3-chloropropyne	[624-65-7]	1.434	7.56	1.67	0.346	0.766	0.42
333	pentafluorobenzene	[363-72-4]	1.391	4.36	1.44	0.319	0.627	0.31
334	ethynylbenzene; phenylacetylene	[536-74-3]	1.548[p]	2.99[p]	0.66	0.412	0.499	0.09
335	ethyl propiolate	[623-47-2]	1.411	7.00		0.331	0.750	0.42
336	1-hexyne	[693-02-7]	1.399[h]		0.86	0.324		
337	1-nonyne	[3452-09-3]	1.422	2.52		0.338	0.432	0.09
Miscellaneous								
338	carbon dioxide (in its supercritical state, at 40°C and several pressures)	[124-38-9]						
339	carbon disulfide	[75-15-0]	1.627[j]	2.643[j]	0.00	0.452	0.451	0.00
340	phosphorus oxychloride; phosphoryl chloride	[10025-87-3]	1.460	13.50	2.54	0.361	0.862	0.50
341	1,1,3,3-tetramethylguanidine	[80-70-6]	1.466 (25°C)[h]	23.1		0.365	0.917	0.55
342	isopropyl nitrate	[1712-64-7]	1.391[h]			0.319		
343	3-methyl-2-oxazolidinone; 3-methyloxazolidin-2-one	[19836-78-3]	1.454[h]	79.3[h]	4.1[n]	0.358	0.975	0.62
344	3-methyl-1,2,3-oxadiazolium-5-olate; 3-methylsydnone (40°C)	[6939-12-4]	1.516 (25°C)[h]			0.394		
345	3-n-propyl-1,2,3-oxadiazolium-5-olate; 3-n-propylsydnone	[6939-15-7]	1.497 (25°C)[h]			0.383		
346	(+)-(2S,3S)-1,4-bis(dimethylamino)-2,3-dimethoxybutane (DDB)	[26549-21-3]	1.434[h]			0.346		

(a) Chemical Abstracts Registry Number of the solvent; (b) Refractive index of the solvent, measured at 20.0 °C, unless noted otherwise. All values taken from [17a], unless noted otherwise; (c) Relative permittivity of the solvent measured at 20.0 °C, unless noted otherwise. All values taken from [17a], unless noted otherwise; (d) Molecular dipole moment of the solvent measured in the gas phase unless noted otherwise. All values in Debye units, taken from [21–23], unless noted otherwise; (e) Function of the refractive index of the solvent defined through the equation $f(n) = (n^2 - 1)/(n^2 + 1)$. See text; (f) Function of the relative permittivity of the solvent defined through the equation $g(\varepsilon_r) = (\varepsilon_r - 1)/(\varepsilon_r + 1)$. See text; (g) Difference between the function $g(\varepsilon_r)$ and $f(n)$; (h) Values taken from [19] and the original publications reported therein; (i) Value taken from *Catálogo de Química Fina 1994–1995*, from Aldrich; (j) Values taken from [20]; (k) Value measured in cyclohexane solution; (l) Value measured as 'pure' liquid; (m) Value measured in tetrachloromethane solution; (n) Value measured in benzene solution; (o) Value measured in n-heptane solution; (p) Value taken from [17b]; (q) Value measured in n-hexane solution; (r) Estimated value, taken from [17b]; (s) Value measured in dioxane solution; (t) 1.13 and 1.36D are the values corresponding to the N-*gauche* and N-*cis* forms, respectively; (u) 0.66 and 0.80D are the values corresponding to the axial and equatorial forms, respectively.

Table 1b

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
gas							
Perfluorinated Solvents							
nonaromatic							
1	perfluoro-n-hexane	338.05	1.677[g]	201.6	30.85[g]	28.37	11.9
2	perfluoro-n-heptane	388.05	1.720[g]	225.6			
3	perfluoro-n-octane	438.06	1.759[g]	249.0	41.13[g]	38.65	12.5
4	perfluoro(methylcyclohexane)	350.05	1.788[g]	195.8	33.95[g]	31.47	12.7
5	perfluorodecalin; perfluorodecahydronaphthalene	462.07	1.937[g]	238.5	45.40[g]	42.92	13.4
6	perfluoro(1-methyldecalin); perfluoro(1-methyldecahydronaphthalene)	512.09	1.950[h]	262.6			
7	perfluorodimethyldecalin	562.10					
8	perfluorotri-n-butylamine; heptacosafluorotributylamine	671.10	1.884	356.2	55.44[i]	52.96	12.2
aromatic							
9	hexafluorobenzene; perfluorobenzene	186.06	1.607	115.8	35.82	33.34	17.0
Cyclic and Acyclic Nonaromatic Hydrocarbons and Related Compounds							
10	2-methylbutane; isopentane	72.15	0.614	117.5	25.22	22.74	13.9
11	n-pentane	72.15	0.621	116.2	26.75	24.27	14.5
12	n-hexane	86.18	0.655	131.6	31.73	29.25	14.9
13	n-heptane	100.20	0.679	147.6	36.66	34.18	15.2
14	n-octane	114.23	0.699	163.4	41.53	39.05	15.5
15	2,2,4-trimethylpentane; isooctane; isobutyltrimethylmethane	114.23	0.688	166.0	35.24	32.76	14.0
16	n-nonane	128.26	0.714	179.6	46.43	43.95	15.6
17	n-decane	142.28	0.726	196.0	51.39	48.91	15.8
18	n-undecane	156.31	0.737[g]	212.1	56.43	53.95	16.0
19	n-dodecane	170.34	0.745	228.6	61.51	59.03	16.1
20	n-pentadecane	212.42	0.765[g]	277.7	76.11	73.63	16.3
21	n-hexadecane	226.45	0.770[g]	294.1	81.38	78.90	16.4
22	cyclopentane; pentamethylene	70.13	0.740	94.8	28.72	26.24	16.6
23	cyclohexane; hexahydrobenzene; hexamethylene	84.16	0.774	108.7	33.12	30.64	16.8
24	cycloheptane	98.19	0.807[g]	121.7	38.56[g]	36.08	17.2
25	cyclooctane	112.22	0.832[g]	134.9	43.38[g]	40.90	17.4
26	methylcyclohexane; hexahydrotoluene; cyclohexylmethane	98.19	0.765	128.4	35.44	32.96	16.0
27	1-hexene	84.16	0.668	126.0	30.63[i]	28.15	14.9
28	cyclohexene; tetrahydrobenzene	82.15	0.806	101.9	33.57	31.09	17.5
29	1,4-cyclohexadiene	80.13	0.851[g]	94.2	34.30[g]	31.82	18.4
30	cycloheptatriene; cyclohepta-1,3,5-triene	92.14	0.887[g]	103.9	38.73[g]	36.25	18.7
31	1,5-cyclooctadiene	108.18	0.880[g]	122,9	43.39	40.91	18.2
32	cyclooctatetraene; 1,3,5,7-cyclooctatetraene	104.15	0.918[g]	113.5	42.20[g]	39.72	18.7
33	trans,trans,cis,-1,5,9-cyclododecatriene	162.28	0.890[g]	182.3	74.68[g]	72.20	19.9
34	dicyclopentadiene; 3a,4,7,7a-tetrahydro-1H-4,7-methano-indene	132.21	0.976[g]	135.5	38.52[g]	36.04	16.3
35	cis-decalin; cis-decahydronaphthalene; cis-bicyclo[4.4.0]decane	138.25	0.893	154.8	51.34[i]	48.86	17.8
36	perhydrofluorene; dodecahydrofluorene	178.32	0.947[g]	188.3	55.25[g]	52.77	16.7
37	quadricyclane; quadricyclo[2.2.1.0^{2,6}.0^{3,5}]heptane	92.14	0.880[g]	104.7	37.0[g]	34.52	18.2
38	tetramethylsilane	88.23	0.637[g]	138.5	26.17[g]	23.69	13.1

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
Aromatic Hydrocarbons							
39	benzene	78.11	0.874	89.4	33.92	31.44	18.8
40	toluene; methyl benzene	92.14	0.862	106.9	38.06	35.58	18.2
41	o-xylene; 1,2-dimethylbenzene	106.17	0.876	121.2	43.45	40.97	18.4
42	m-xylene; 1,3-dimethylbenzene	106.17	0.860	123.5	42.68	40.20	18.0
43	p-xylene; 1,4-dimethylbenzene	106.17	0.857	123.9	42.42	39.94	18.0
44	mesitylene; 1,3,5-trimethylbenzene	120.19	0.861	139.6	47.51	45.03	18.0
45	prehnitene; 1,2,3,4-tetramethylbenzene	134.22	0.901^g	149.0	45.02^g	42.54	16.9
46	ethylbenzene; phenylethane	106.17	0.863	123.0	42.26	39.78	18.0
47	cumene; isopropyl benzene; 2-phenylpropane; 1-methylethylbenzene	120.19	0.857	140.2	45.14	42.66	17.4
48	cyclohexylbenzene; phenylcyclohexane	160.26	0.939	170.7	59.94^g	57.46	18.3
49	diphenylmethane; 1,1′-methylenebis-benzene; methyl-1,1′-biphenyl	168.24	1.006^g	167.2	67.49^g	65.01	19.7
50	1-methylnaphthalene	142.20	1.017	139.8	60.07^i	57.59	20.3
51	tetralin; 1,2,3,4-tetrahydronaphthalene	132.21	0.966	136.9	55.23^i	52.75	19.6
Halogenated Compounds							
nonaromatic							
52	carbon tetrachloride; tetrachloromethane	153.82	1.584	97.1	32.54	30.06	17.6
53	fluorotrichloromethane; trichlorofluoromethane	137.37	1.476	93.1	25.02^i	22.54	15.6
54	bromotrichloromethane	198.28	2.000^g	99.1			
55	1,1-dichloroethane; ethylidene chloride	98.96	1.168	84.7	30.77	28.29	18.3
56	1,2-dichloroethane; ethylene chloride	98.96	1.246	79.4	35.22	32.74	20.3
57	1,1,1-trichloroethane; methyl chloroform	133.41	1.330	100.3	32.62	30.14	17.3
58	1,1,2-trichloroethane	133.41	1.432	93.2	40.28	37.80	20.1
59	1,1,1-trichlorotrifluoroethane	187.38	1.566^g	119.7	28.32	25.84	14.7
60	1,1,2-trichloro-1,2,2-trifluoroethane	187.38	1.564	119.8	28.61	26.13	14.8
61	1,1-dichloroethylene; 1,1-dichloroethene	96.94	1.175	82.5	26.74	24.26	17.2
62	cis-1,2-dichloroethylene; cis-1,2-dichloroethene	96.94	1.276	76.0	31.80^g	29.32	19.6
63	trans-1,2-dichloroethylene; trans-1,2-dichloroethene	96.94	1.246	77.8	29.29^g	26.81	18.6
64	trichloroethylene; trichloroethene	131.39	1.460	90.0	34.62	32.14	18.9
65	tetrachloroethylene; tetrachloroethene; ethylene tetrachloride	165.83	1.614	102.7	39.72	37.24	19.0
66	1-chloropropane; n-propyl chloride	78.54	0.883	88.9	28.56	26.08	17.1
67	1,3-dichloropropane; trimethylene chloride	112.99	1.179^g	95.8	40.79	38.31	20.0
68	2,2-dichloropropane; isopropylidene chloride	112.99	1.084^g	104.2	31.90^g	29.42	16.8
69	3-chloro-1,1,1-trifluoropropane	132.51	1.326 (20 °C)^g	99.9	29.29^g	26.81	16.4
70	1,2-dichloro-1,1,2,3,3,3-hexafluoropropane	220.93	1.571^g	140.6	27.30	24.82	13.3
71	1,2,3-trichloropropane; glycerin trichlorohydrin	147.43	1.383	106.6	46.94^i	44.46	20.4
72	hexachloropropene	248.75	1.760^g	141.3			
73	1-chlorobutane; n-butyl chloride	92.57	0.881	105.1	33.63	31.15	17.2
74	1,4-dichlorobutane; tetramethylen chloride	127.01	1.134^g	112.0	46.36	43.88	19.8

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
75	hexachloro-1,3-butadiene	260.76	1.682 (20 °C)^g	155.0			
76	1,2-dichloro-1,2,3,3,4,4-hexafluorocyclobutane	232.94					
77	hexachlorocyclopentadiene	272.77	1.702^g	160.3			
78	chlorocyclohexane; cyclohexyl chloride	118.61	0.994^g	119.3	42.92^g	40.40	18.4
79	1,10-dichlorodecane; decamethylen chloride	211.18	0.995^g	212.2	80.07^g	77.59	19.1
80	methyltrichlorosilane; trichloromethylsilane	149.48	1.269^g	117.8	30.31^g	27.83	15.4
81	bromoethane; ethyl bromide	108.97	1.451	75.1	28.26	25.78	18.5
82	1,2-dibromoethane; ethylene bromide	187.86	2.169	86.6	41.74	39.26	21.3
83	1-bromopropane; n-propyl bromide	123.00	1.345	91.4	32.13	29.65	18.0
84	1-bromobutane; n-butyl bromide	137.02	1.269	108.0	36.71	34.23	17.8
85	iodomethane; methyl iodide	141.94	2.265	62.7	27.97^i	25.49	20.2
86	diiodomethane; methylene iodide	267.84	3.308	81.0	49.38^i	46.90	24.1
87	iodoethane; ethyl iodide	155.97	1.924	81.1	32.05	29.57	19.1
88	1-iodopropane; n-propyl iodide	169.99	1.739	97.8	36.32	33.84	18.6
89	2-iodopropane; isopropyl iodide	169.99	1.695	100.3	34.06^i	31.58	17.7
90	1-iodobutane; n-butyl iodide	184.02	1.607	114.5	40.67	38.19	18.3
aromatic							
91	fluorobenzene; phenyl fluoride	96.10	1.019	94.3	34.68	32.20	18.5
92	1,2-difluorobenzene	114.09	1.150^g	99.2	36.24	33.76	18.4
93	1,3-difluorobenzene	114.09	1.147^g	99.5	34.69	32.21	18.0
94	1,4-difluorobenzene	114.09	1.163^g	98.1	35.62	33.14	18.4
95	1,3,5-trifluorobenzene	132.09	1.277 (20 °C)^g	103.4			
96	(trifluoromethyl)benzene; α,α,α-trifluorotoluene	146.11	1.184^g	123.4	37.67	35.19	16.9
97	2,3,4,5,6-pentafluorotoluene	182.09	1.436^g	126.8	41.13	38.65	17.5
98	chlorobenzene; phenyl chloride	112.56	1.101	102.2	41.00	38.52	19.4
99	1,2-dichlorobenzene	147.00	1.300	113.1	50.21^i	47.73	20.5
100	1,3-dichlorobenzene	147.00	1.283	114.6	48.58^i	46.10	20.1
101	1,4-dichlorobenzene	147.00	1.283	114.6	49.0^i	46.52	20.1
102	1,2,3-trichlorobenzene	181.45	1.472^g	123.3			
103	1,2,4-trichlorobenzene	181.45	1.448^g	125.3	54.36^g	51.88	20.3
104	1,2,3,4-tetrachlorobenzene	215.89	1.858^g	116.2	60.84^g	58.36	22.4
105	1-chloronaphthalene; 1-naphthyl chloride	162.62	1.189^g	136.8			
106	bromobenzene; phenyl bromide	157.01	1.488	105.5	44.54	42.06	20.0
107	1,2-dibromobenzene	235.92	1.976^g	119.4	55.14^g	52.66	21.0
108	1,3-dibromobenzene	235.92	1.947^g	121.2			
109	2,5-dibromotoluene	219.94	1.815^g	137.7			
110	iodobenzene; phenyl iodide	204.01	1.823	111.9	49.58^i	47.10	20.5
111	1-iodonaphthalene; 1-naphthyl iodide	254.07	1.734^g	146.5	70.34^g	67.86	21.5
Nitriles							
112	acetonitrile; ethanenitrile; methyl cyanide; cyanomethane	41.05	0.776	52.9	33.40	30.92	24.2
113	propionitrile; propanenitrile; ethyl cyanide	55.08	0.777	70.9	36.19	33.71	21.8
114	butyronitrile; butanenitrile; n-propyl cyanide; 1-cyanopropane	69.11	0.787	87.8	39.41	36.93	20.5
115	valeronitrile; pentanenitrile; n-butyl cyanide	83.13	0.795	104.6	43.64	41.16	19.8
116	hexanenitrile; capronitrile; n-amyl cyanide; n-pentyl cyanide	97.16	0.801	121.3	47.91	45.43	19.4
117	undecanenitrile; decyl cyanide	167.30	0.818^g	204.5	71.14	68.66	18.3
118	dodecanenitrile; undecyl cyanide; lauronitrile	181.32	0.820^g	221.1	76.12	73.64	18.2

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H°^{\ d}$	$\Delta_{vap}U°^{\ e}$	$\delta_H^{\ f}$
119	chloroacetonitrile; chloroethanenitrile	75.50	1.189^g	63.5			
120	trichloroacetonitrile; trichloroethanenitrile	144.39	1.440^g	100.3	34.16^g	31.68	17.8
121	pivalonitrile; 2,2-dimethylpropanenitrile; tert-butyl cyanide;trimethylacetonitrile	83.13	0.758^g	109.7	37.50	35.02	17.9
122	3-methoxypropanenitrile	85.11	0.936^g	90.9			
123	acrylonitrile; 2-propenenitrile; vinyl cyanide; cyanoethylene	53.06	0.800	66.3	32.64^i	30.16	21.3
124	benzonitrile; phenyl cyanide; cyanobenzene	103.12	1.001	103.0	55.48^i	53.00	22.7
125	phenylacetonitrile; benzyl cyanide; benzeneacetonitrile	117.15	1.014^g	115.5	52.15^g	49.67	20.7
126	N,N-dimethylcyanamide; dimethyl-carbamonitrile	70.09	0.889 (20 °C)^g	78.8			
127	N,N-diethylcyanamide; diethyl-carbamonitrile	98.15	0.860^g	114.1			
128	N,N-diisopropylcyanamide; diisopropyl-carbamonitrile	126.20	0.949^g	133.0			
Ethers and Orthoesters							
129	diethyl ether; ethyl ether; ethoxyethane; 1,1′-oxybisethane	74.12	0.708	104.7	27.37	24.89	15.4
130	di-n-propyl ether; n-propyl ether; 1,1′-oxybispropane	102.18	0.742	137.7	35.79	33.31	15.6
131	diisopropyl ether; isopropyl ether; 2,2′-oxybispropane	102.18	0.719	142.1	32.26	29.78	14.5
132	di-n-butyl ether; n-butyl ether	130.23	0.764	170.5	45.00	42.52	15.8
133	di-tert-butyl ether; tert-butyl ether	130.23	0.759^g	171.6	37.69	35.21	14.3
134	diphenyl ether; phenyl ether; 1,1′-oxybisbenzene; diphenyl oxide; phenoxybenzene	170.21	1.070	159.1	66.90^i	64.42	20.1
135	dibenzyl ether; benzyl ether; 1,1′-[oxybis(methylene)]bisbenzene	198.26	1.040	190.6			
136	n-butyl methyl ether; 1-methoxybutane	88.15	0.739^g	119.3	32.53	30.05	15.9
137	tert-butyl methyl ether; 2-methoxy-2-methylpropane	88.15	0.735^g	119.9	30.04	27.56	15.2
138	tert-butyl ethyl ether; 2-ethoxy-2-methylpropane	102.18	0.736^g	138.8	32.97	30.49	14.8
139	tert-amyl methyl ether; 2-methoxy-2-methylbutane	102.18	0.766^g	133.4	33.37^g	30.89	15.2
140	ethyl vinyl ether; ethoxyethene	72.11	0.749^g	96.3	27.5^i	25.02	16.1
141	anisole; methyl phenyl ether; methoxybenzene	108.14	0.989	109.3	46.91	44.43	20.2
142	phenetole; ethyl phenyl ether; ethoxybenzene	122.17	0.960	127.3	51.04^i	48.56	19.5
143	cineole; 1,3,3-trimethyl-2-oxabicyclo[2,2,2]octane	154.25	0.919	167.8			
144	bis(2-chloroethyl) ether; 1,1′-oxybis[2-chloroethane]; 2,2′-dichlorodiethyl ether	143.01	1.213	117.0			
145	dimethoxymethane; methylal	76.10	0.854	89.1	28.89^i	26.41	17.2
146	diethoxymethane	104.15	0.825^g	126.2	35.74	33.26	16.2
147	ethylene glycol dimethyl ether; 1,2-dimethoxyethane;monoglyme	90.12	0.864	104.3	36.47	33.99	18.1
148	diethylene glycol dimethyl ether; bis(2-methoxyethyl) ether; diglyme; 1,1′-oxybis[2-methoxyethane]	134.18	0.938	142,9	44.70	42.22	17.2
149	triethylene glycol dimethyl ether; triglyme	178.23	0.981^g	181.7			

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
150	diethylene glycol diethyl ether; bis(2-ethoxyethyl) ether; 1,1'-oxybis(2-ethoxyethane)	162.23	0.904^g	179.5	58.40	55.92	17.7
151	1,2-dimethoxybenzene; veratrole	138.17	1.082	127.7			
152	trimethyl orthoformate; trimethoxymethane	106.12	0.963^g	110.2			
153	trimethyl orthoacetate; 1,1,1-trimethoxyethane	120.15	0.944^g	127.3	39.20^g	36.72	17.0
154	furan; oxole; furfuran	68.08	0.931	73.1	27.71	25.23	18.6
155	tetrahydrofuran; oxolane; oxacyclopentane; diethylene oxide; tetramethylene oxide	72.11	0.881	81.9	32.16	29.68	19.0
156	2-methyltetrahydrofuran; 1,4-oxidopentane	86.13	0.847^g	101.7			
157	2,5-dimethyltetrahydrofuran (cis + trans)	100.16	0.833^g	120.2	35.02^g	32.54	16.5
158	2,2,5,5-tetramethyltetrahydrofuran	128.22	0.807^g	158.9			
159	tetrahydropyran; oxane; pentamethylene oxide; oxacyclohexane	86.13	0.877	98.2	34.67	32.19	18.1
160	(±)-3-methyltetrahydropyran	100.16	0.860 (20 °C)^g	116.5			
161	1,4-dioxane; p-dioxane; diethylene dioxide	88.11	1.028	85.7	38.66	36.18	20.5
162	1,3-dioxolane; ethylene glycol methylene ether	74.08	1.059^g	70.0	35.60^i	33.12	21.8
163	5-acetyl-5-methyl-1,3-dioxane	144.17	1.087 (20 °C)^g	132.6			
164	2-methoxy-1,3-dioxolane	104.11	1.092^h	95.3			
165	(±)-methyloxirane; propylene oxide	58.08	0.825^g	70.4	28.31	25.83	19.2
166	(±)-chloromethyl)oxirane; epichlorohydrin; 1-chloro-2,3-epoxypropane	92.53	1.175	78.7			

Acyl Compounds
ketones

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
167	acetone; 2-propanone; dimethyl ketone	58.08	0.784	74.1	31.27	28.79	19.7
168	2-butanone; methyl ethyl ketone	72.11	0.800	90.1	34.92	32.44	19.0
169	3-methyl-2-butanone; isopropyl methyl ketone	86.13	0.804^g	107.1	36.87	34.39	17.9
170	3,3-dimethyl-2-butanone; tert-butyl methyl ketone; pinacolone	100.16	0.807^g	124.1	38.00	35.52	16.9
171	2-pentanone; n-propyl methyl ketone	86.13	0.802	107.4	38.46	35.98	18.3
172	3-pentanone; diethyl ketone	86.13	0.809	106.5	38.68	36.20	18.4
173	4-methyl-2-pentanone; isobutyl methyl ketone	100.16	0.796	125.8	40.65	38.17	17.4
174	2,4-dimethyl-3-pentanone; diisopropyl ketone	114.19	0.799	142.9	41.57	39.09	16.5
175	2,2,4,4-tetramethyl-3-pentanone; di-tert-butyl ketone	142.24	0.820^g	173.5	45.40	42.92	
176	2~hexanone; methyl n-butyl ketone	100.16	0.807	124.1	43.15	40.67	18.1
177	4-heptanone; di-n-propyl ketone	114.19	0.815^g	140.1	46.74^g	44.26	17.8
178	2,6-dimethyl-4-heptanone; diisobutyl ketone; isovalerone	142.24	0.801	177.4	50.92	48.44	16.5
179	5~nonanone; di-n-butyl ketone	142.24	0.818^g	173.9	53.30	50.82	17.1
180	cyclopentanone	84.12	0.944	89.1	42.77	40.29	21.3
181	cyclohexanone; cyclohexyl ketone	98.14	0.942	104.2	45.09	42.61	20.2
182	cyclopropyl methyl ketone; cyclopropylmethylmethanone	84.12	0.897^g	93.8	39.95^g	37.47	20.0

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	$\delta_H^{\ f}$
183	dicyclopropyl ketone; dicyclopropylmethanone	110.16	0.968 (20 °C)[g]	113.8	53.70[g]	51.22	21.2
184	acetophenone; acetylbenzene; 1-phenylethanone; methyl phenyl ketone	120.15	1.024	117.3	53.39[i]	50.91	20.8
185	2,4-pentanedione; acetylacetone	100.12	0.972	103.0	41.78	39.30	19.5
186	1,1,1-trichloroacetone	161.42	1.428[g]	113.04			
187	hexachloroacetone	246.75	1.732[g]	142.5			
188	1,1,1-trichloro-3,3,3-trifluoroacetone	215.39					

esters, lactones, anhydrides

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	$\delta_H^{\ f}$
189	methyl formate; methyl methanoate	60.05	0.967	62.2	28.60	26.12	20.5
190	methyl acetate; methyl ethanoate	74.08	0.928	79.8	32.50	30.02	19.4
191	methyl propionate; methyl propanoate	88.11	0.908[g]	97.0	35.95	33.47	18.6
192	methyl butyrate; methyl butanoate	102.13	0.891[g]	114.6	39.33	36.85	17.9
193	methyl valerate; methyl pentanoate	116.16	0.885[g]	131.3	43.13	40.65	17.6
194	methyl caproate; methyl hexanoate	130.19	0.880[g]	147.9	48.04	45.56	17.6
195	methyl caprylate; methyl octanoate	158.24	0.872[g]	181.5	56.41	53.93	17.2
196	methyl caprate; methyl decanoate	186.30	0.869[g]	214.4	66.75	64.27	17.3
197	methyl laurate; methyl dodecanoate	214.35	0.866[g]	247.5	77.17	74.69	17.4
198	methyl oleate; methyl (Z)-9-octadecenoate	296.49	0.870	340.8	106.82[i]	104.34	17.5
199	methyl linoleate	294.48	0.884[g]	333.1			
200	methyl acrylate; methyl 2-propenoate	86.09	0.951	90.5	29.20[g]	26.72	17.2
201	methyl methacrylate; methyl 2-methyl-2-propenoate	100.17	0.938	106.8	40.7[i]	38.22	18.9
202	methyl benzoate; methyl benzenecarboxylate	136.15	1.084	125.6	55.57	53.09	20.6
203	methyl trifluoroacetate; methyl trifluoroethanoate	128.05	1.283 (20 °C)[g]	99.8			
204	methyl trichloroacetate	177.42	1.480[g]	229.9	48.34	45.86	19.6
205	ethyl formate; ethyl methanoate	74.08	0.915	81.0	32.11	29.63	19.1
206	ethyl acetate; ethyl ethanoate	88.11	0.895	98.4	35.69	33.21	18,4
207	ethyl acetoacetate; ethyl acetoethanoate; ethyl 3-oxobutanoate	130.14	1.021	127.5			
208	ethyl lactate; ethyl 2-hydroxypropionate	118.13	1.027	115.0	49.4[i]	46.92	20.2
209	ethyl benzoate; ethyl benzenecarboxylate	150.18	1.042	144.1	40.5[i]	38.02	16.2
210	ethyl chloroacetate; ethyl chloroethanoate	122.55	1.145[g]	107.0	49.48	47.00	21.0
211	ethyl trichloroacetate; ethyl trichloroethanoate	191.44	1.376[g]	139.1	50.97	48.49	18.7
212	n-propyl formate; n-propyl methanoate	88.11	0.900	97.9	37.61	35.13	18.9
213	n-propyl acetate; n-propyl ethanoate	102.13	0.883	115.7	39.77	37.29	18.0
214	n-butyl acetate; n-butyl ethanoate	116.16	0.876	132.6	43.89	41.41	17.7
215	isoamyl acetate; isopentyl acetate; 3-methyl-1-butyl acetate	130.19	0.866	150.3			
216	vinyl acetate; vinyl ethanoate; ethenyl acetate	86.09	0.925	93.1	34.38[g]	31.90	18.5
217	dimethyl carbonate; methyl carbonate	90.08	1.063[g]	84.7	34.54[g]	32.06	19.5
218	diethyl carbonate; ethyl carbonate	118.13	0.969	121.9	43.60	41.12	18.4
219	diethyl malonate; ethyl malonate; diethyl propanedioate	160.17	1.050	152.5			

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
220	1,3-dioxolan-2-one; ethylene carbonate; cyclic ethylene carbonate	88.06	1.338	65.8			
221	4,5-dichloro-1,3-dioxolan-2-one	156.95	1.590^g	98.7			
222	(±)-propylene carbonate; 4-methyl-1,3-dioxolan-2-one	102.09	1.199^g	85.1	65.31 (20 °C)^g	62.83	27.2
223	γ-butyrolactone; 2(3H)-dihydrofuranone; 4-hydroxybutyric acid γ-lactone	86.09	1.125	76.5			
224	δ-valerolactone; tetrahydropyran-2-one	160.12	1.103^g	145.2	58.00^g	55.52	19.6
225	acetic anhydride; acetic acid anhydride; ethanoic anhydride	102.09	1.075	95.0			
226	trichloroacetic anhydride	308.76	1.690^g	182.7			
227	triacetin; glyceryl triacetate; 1,2,3-propanetriol triacetate	218.21	1.153	189.3	85.74	83.26	21.0
228	triolein; 1,2,3-propanetriyl-tri-(Z)-9-octadecenoate; glycerol trioleate	885.45	0.915^g	967.7			
229	dimethyl phthalate	194.19	1.187^g	163.6	75.78^g	73.30	21.2
230	di-n-butyl phthalate	278.35	1.043^g	266.9	96.72^g	94.24	18.8
Di-substituted Amides and Thioamides and Tetrasubstituted Ureas							
231	N,N-dimethylformamide (DMF)	73.09	0.944	77.4	46.88	44.40	24.0
232	N,N-dimethylacetamide	87.12	0.936	93.1	50.24	47.76	22.6
233	N,N-dimethylpropionamide; ethyl-N,N′-dimethyl formamide	101.15	0.920^g	109.9			
234	N,N-diethylformamide	101.15	0.903^g	112.0	50.32	47.84	20.7
235	N,N-diethylacetamide	115.18	0.904^g	127.4	54.11	51.63	20.1
236	N,N-dimethylthioformamide; thioformyldimethylamine	89.16	1.024 (27 °C)^g	87.1			
237	N-methylformanilide	135.17	1.092^g	123.8			
238	1,1,3,3-tetramethylurea	116.16	0.962	120.7			
239	1,1,3,3-tetraethylurea	172.27	0.903^g	190.8			
240	1-formylpiperidine; piperidine-1-carbaldehyde; 1-piperidinecarboxaldehyde	113.16	1.019^g	111.1			
241	1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidone; N,N′-dimethyl-N,N′-trimethyleneurea (DMPU)	128.18	1.060^g	120.9			
242	1-methyl-2-pyrrolidinone; N-methylpyrrolidone	99.13	1.026	96.6	52.80^i	50.32	22.8
243	1-methylpyrrolidine-2-thione	115.19					
244	1-ethyl-2-pyrrolidone; 1-ethyl-pyrrolidin-2-one	113.16	0.998 (20 °C)^g	113.4			
245	1-cyclohexyl-2-pyrrolidone; 1-cyclohexyl-pyrrolidin-2-one	167.25	1.007^h	112.4			
246	1-methylhexahydroazepin-2-one; N-methyl-ε-caprolactam; 1-methyl-azepan-2-one	127.19	1.013 (20 °C)^j	125.6			
247	pyrrolidine-1-carbonitrile; N-cyanopyrrolidine	96.13	0.954^h				
248	piperidine-1-carbonitrile; N-cyanopiperidine	110.16	0.951^h				
249	morpholine-4-carbonitrile; N-cyanomorpholine	112.12	1.109^h				
Phosphates, HMPA							
250	trimethyl phosphate; phosphoric acid trimethyl ester; methyl phosphate	140.08	1.205	116.2	47.3^i	44.82	19.6

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
251	triethyl phosphate; phosphoric acid triethyl ester; ethyl phosphate	182.16	1.068	170.6	57.3[i]	54.82	17.9
252	tri-n-propyl phosphate; phosphoric acid tripropyl ester; propyl phosphate	224.24	1.005[g]	223.1			
253	tri-n-butylphosphate; phosphoric acid tributyl ester; butyl phosphate	266.32	0.976	272.9			
254	diethylchlorophosphate; phosphorochloridic acid diethyl ester; diethyl phosphorochloridate	172.55	1.200 (20 °C)[g]	143.8			
255	hexamethylphosphorictriamide; hexamethylphosphoramide (HMPA)	179.20	1.020	175.7	61.1[i]	58.62	18.3
256	hexamethylphosphorothioic acid triamide (HMPTA)	195.26	1.044[g]	187.0			
257	methylphosphonic acid bis(dimethylamide)	150.16	1.016[g]	147.8			

Sulfates, Sulfites, Sulfoxides, Sulfamides

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
258	dimethyl sulfate; sulfuric acid dimethyl ester	126.13	1.322[g]	95.4	48.53[g]	46.05	22.0
259	dimethyl sulfite; methyl sulfite; sulfurous acid dimethyl ester	110.13	1.207[g]	91.2	40.17	37.69	20.3
260	diethyl sulfite; ethyl sulfite; sulfurous acid diethyl ester	138.19	1.077[g]	128.3	48.53[g]	46.05	18.9
261	dimethyl sulfoxide (DMSO); methyl sulfoxide; sulfinylbismethane	78.13	1.095	71.4	52.88[i]	50.40	26.6
262	tetramethylene sulfoxide; tetrahydrothiophene-1-oxide	104.17	1.168[g]	89.2			
263	sulfolane; tetramethylene sulfone; tetrahydrothiophene 1,1-dioxide	120.17	1.264	95.1			
264	methyl methylthiomethyl sulfoxide; methylmethylsulfinylmethyl sulfide; methanesulfinyl-methylsulfonyl-methane	124.22	1.216[g]	102.2			
265	3-methyltetrahydrothiophene-1,1-dioxide; 3-methylsulfolane	134.20	1.189[g]	112.9			
266	N,N,N′,N′-tetraethylsulfamide	208.33	1.037[g]	200.9			

Pyridines

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
267	pyridine; azine	79.10	0.978	80.9	40.21	37.73	21.6
268	2-picoline; 2-methylpyridine	93.13	0.940	99.1	42.51	40.03	20.1
269	4-picoline; 4-methylpyridine	93.13	0.950	98.0	44.83	42.35	20.8
270	2,6-lutidine; 2,6-dimethylpyridine	107.16	0.918	116.7	45.38	42.90	19.2
271	3,4-lutidine; 3,4-dimethylpyridine	107.16	0.954[g]	112.3	50.54	48.06	20.7
272	2,4,6-collidine; 2,4,6-trimethylpyridine	121.18	0.910	133.2	50.34	47.86	19.0
273	2,6-di-tert-butylpyridine	191.32	0.852[h]	224.6	56.52[g]	54.04	15.5
274	2-cyanopyridine; 2-pyridinecarbonitrile	104.11	1.081[g]	96.3	73.64[g]	71.16	27.2
275	2-fluoropyridine	97.09	1.123[g]	86.5	43.54[g]	41.06	21.8
276	2,6-difluoropyridine	115.08	1.268[h]	90.8			
277	pentafluoropyridine; perfluoropyridine	169.05	1.540[h]	109.8	36.34[g]	33.86	17.6
278	2-chloropyridine	113.55	1.203[g]	94.4	47.15[g]	44.67	21.8
279	2-bromopyridine	158.00	1.610[g]	98.1	51.08[g]	48.60	22.3
280	3-bromopyridine	158.00	1.613[g]	98.0	45.22[g]	42.74	20.9
281	pyrimidine	80.09	1.079[g]	74.2	49.81	47.33	25.3
282	quinoline	129.16	1.090	118.5	57.36[g]	54.88	21.5

Tertiary Amines

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	δ_H^f
283	triethylamine; N,N-diethylethanamine	101.19	0.723	140.0	34.96	32.48	15.2

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	$\delta_H^{\ f}$
284	tri-n-butylamine; N,N-dibutyl-1-butanamine	185.35	0.774	239.5			
285	N,N-dimethylcyclohexylamine	127.23	0.849^h	149.9			
286	N,N-dimethylbenzylamine	135.21	0.901^g	150.1			
287	N,N-dimethylaniline; N,N-dimethylbenzenamine	121.18	0.952	127.3	49.8^i	47.32	19.3
288	1-methylpiperidine	99.18	0.816^g	121.5	36.72^g	34.24	16.8
289	1-methylimidazole	82.11	1.029^g	79.8	54.64^g	52.16	25.6
290	1,4-dimethylpiperazine	114.19	0.856^g	133.4			
Sulfides and Disulfides							
291	dimethyl sulfide; methyl sulfide; thiobismethane; 2-thiapropane	62.13	0.842	73.8	27.99	25.51	18.6
292	diethyl sulfide; ethyl sulfide; 1,1′-thiobisethane; 3-thiapentane	90.18	0.831	108.5	35.88	33.40	17,5
293	diisopropyl sulfide; isopropyl sulfide; 2,2′-thiobispropane	118.24	0.810^g	146.0	39.64	37.16	19.0
294	di-n-butyl sulfide; n-butyl sulfide; 1,1′-thiobisbutane	146.29	0.835^g	175.2	52.96	50.48	17.0
295	di-tert-butyl sulfide; tert-butyl sulfide; 2,2′-thiobis(2-methylpropane)	146.29	0.815^h	179.5	43.93^g	41.45	15.2
296	dimethyl disulfide; methyl disulfide	94.19	1.056^g	89.2	37.90	35.42	19.9
297	diethyl disulfide; ethyl disulfide	122.25	0.988^g	123.7	45.20	42.72	18.6
298	trimethylene sulfide; thiacyclobutane	74.15	1.016^g	73.0	36.01	33.53	21.4
299	thiophene; thiofuran; thiofurfuran	84.14	1.059	79.5	34.79	32.31	20.2
300	tetrahydrothiophene; thiacyclopentane; diethylene sulfide	88.17	0.994	88.7	39.46	36.98	20.4
301	pentamethylene sulfide; tetrahydrothiopyran; thiacyclohexane	102.20	0.981^g	104.2	42.60	40.12	19.6
302	thioanisole; methylthiobenzene; phenyl methylmethylthiosulfide; phenyl 1-thiaethane	124.21	1.054^g	117.8	50.63^g	48.15	20.2
Nitro Compounds							
303	nitromethane	61.04	1.131	54.0	38.36	35.88	25.8
304	nitroethane	75.07	1.045	71.8	41.59	39.11	23.3
305	2-nitropropane	89.09	0.983	90.6	41.34^i	38.86	20.7
306	2-methyl-2-nitropropane	103.12	0.956^g	107.9	40.17^g	37.69	18.7
307	nitrocyclohexane	129.16	1.061^g	121.7			
308	nitrobenzene	123.11	1.198	102.8	55.01	52.53	22.6
Weak Hydrogen-Bonding Donors							
Primary and secondary amines							
309	n-butylamine; 1-butanamine; 1-aminobutane	73.14	0.737	99.2	35.84	33.36	18.3
310	tert-butylamine; 2-methyl-2-propanamine	73.14	0.691	105.8	29.92	27.44	16.1
311	allylamine; 2-propen-1-amine; 2-propenylamine; 3-aminopropylene	57.10	0.758	75.3			
312	propargylamine; 2-propyn-1-amine	55.08	0.751^g	73.3			
313	diethylamine; N-ethylethanamine	73.14	0.702	104.2	31.47	28.99	16.7
314	diisopropylamine; N-(1-methylethyl)-2-propanamine	101.19	0.710	142.5	34.72	32.24	15.0
315	diallylamine	97.16	0.792 (20 °C)^g	122.7			
316	cyclohexylamine; cyclohexanamine; aminocyclohexane; hexahydroaniline	99.18	0.862	115.1	43.70	41.22	18.9
317	N-methylcyclohexylamine; N-methylcyclohexanamine	113.20	0.868 (23 °C)^g	130.4			
318	piperidine; hexahydropyridine; pentamethylenimine	85.15	0.857	99.4	39.29^i	36.81	19.2

Table 1b *Continued*

No.	Compounds	M^a	$d^{25\ b}$	$V_m^{25\ c}$	$\Delta_{vap}H^{\circ\ d}$	$\Delta_{vap}U^{\circ\ e}$	$\delta_H^{\ f}$
319	morpholine; tetrahydro-2H-1,4-oxazine; diethylene oximide	87.12	0.995	87.6	43.97[i]	41.49	21.8
320	pyrrole; azole	67.09	0.966	69.5	45.37	42.89	24.8
321	1-methylpyrrole	81.12	0.904[g]	89.7	40.71[g]	38.23	20.6
322	N-benzylmethylamine	121.18	0.944 (15 °C)[g]	128.4			
323	N-(tert-butyl)benzylamine	163.27	0.897[g]	182.0			
324	aniline; aminobenzene; phenylamine	93.13	1.018	91.5	55.83	53.35	24.1
325	N-methylaniline; N-methylbenzenamine	107.16	0.982	109.1	53.1[i]	50.62	21.5
CH acids							
326	dichloromethane; methylene chloride	84.93	1.317	64.5	29.00	26.52	20.3
327	chloroform; trichloromethane	119.38	1.480	80.7	31.40	28.92	18.9
328	dibromomethane; methylene bromide	173.85	2.481[g]	70.1	37.03	34.55	22.2
329	bromoform; tribromomethane	252.74	2.878	87.8	46.06	43.58	22.3
330	1,1,2,2-tetrachloroethane; acetylene tetrachloride	167.85	1.587	105.8	45.72	43.24	20.2
331	pentachloroethane	202.30	1.673[g]	120.9	40.61[g]	38.13	17.8
332	propargyl chloride; 3-chloropropyne	74.51	1.024[g]	72.8			
333	pentafluorobenzene	168.06	1.518[g]	110.7	36.36	33.88	17.5
334	ethynylbenzene; phenylacetylene	102.14	0.924[g]	110.5	45.22 (18 °C)[g]	42.74	19.7
335	ethyl propiolate	98.10	0.958[g]	102.4			
336	1-hexyne	82.15	0.710[g]	115.7	31.68[g]	29.20	15.9
337	1-nonyne	124.23	0.753[g]	165.0			
Miscellaneous							
338	carbon dioxide (in its supercritical state, at 40°C and several pressures)	44.01					
339	carbon disulfide	76.14	1.256	60.6	27.65	25.17	20.4
340	phosphorus oxychloride; phosphoryl chloride	153.33	1.645[h]	93.2			
341	1,1,3,3-tetramethylguanidine	115.18	0.914[g]	126.0	46.86[g]	44.38	18.8
342	isopropyl nitrate	105.09	1.030[g]	102.0	38.81[g]	36.33	18.9
343	3-methyl-2-oxazolidinone; 3-methyloxazolidin-2-one	101.11	1.169[g]	86.5			
344	3-methyl-1,2,3-oxadiazolium-5-olate; 3-methylsydnone (40°C)	100.08					
345	3-n-propyl-1,2,3-oxadiazolium-5-olate; 3-n-propylsydnone	128.13	1.158	110.6			
346	(+)-(2S,3S)-1,4-bis (dimethylamino)-2,3-dimethoxybutane (DDB)	176.30	0.896 (20 °C)[g]	196.8			

(a) Molar mass of the solvent, in g/mol; (b) Relative density of the solvent, at 25 °C, unless noted otherwise. It is a dimensionless magnitude. All values taken from ref. [20], unless noted otherwise. (c) Molar volume of the solvent at 25 °C, in cm^3/mol; (d) Standard enthalpy of vaporization of the solvent at 298.15 K, in kJ/mol. All values taken from [24], unless noted otherwise; (e) Standard internal energy of vaporization of the solvent at 298.15 K, in kJ/mol; (f) Cohesive energy density of the solvent in Mpa$^{1/2}$; (g) Values taken from [19] and the original publications reported therein; (h) Value taken from *Catálogo de Química Fina 1994-1995*, from Aldrich. Temperature is not given. (i) Value taken from [20].

DEFINITION, UNITS AND SOURCES OF MODEL-DEPENDENT SCALES

'Overall solvation' scales

E_T (30) and $E_T{}^N$

These are possibly the most widely used empirical solvent 'polarity' scales. According to Reichardt [1,3], the $E_T(30)$ value for a specified solvent is defined as the molar transition energy (in kcal/mol) for the long wavelength electronic transition of dye **1a**, 2,6-diphenyl-4-(2,4,6-triphenylpyridinio)-phenolate as a solution in this solvent at 25.0 °C and at a pressure of 0.1 MPa. $E_T(30)$ is obtained from the experimentally determined vacuum wavelength of the absorption maximum of this transition (λ_{max}) through eqn (11):

$$E_T(30)/(kcal/mol) = 28\,591/(\lambda_{max}/nm) \tag{11}$$

The long-wavelength intramolecular charge-transfer absorption band ('solvatochromic band' [1]) exhibits very large hypsochromic shifts with increasing solvent 'polarity' (in Reichardt's sense).

1a is very sparingly soluble in solvents of low polarity. This has prompted Reichardt and co-workers to develop other indicators endowed with higher solubility in these media. The much more lipophilic penta-*tert*-butyl-substituted derivative **1b** has been found to be quite satisfactory for the purpose of extending the $E_T(30)$ scale to these solvents (Scheme 1). The quantitative link between $E_T(30)$ and $E_T(\mathbf{1b})$ is given by eqn [12]:

$$E_T(\mathbf{1b})/(kcal/mol) = 0.9424 E_T(30)/(kcal/mol) + 1.808 \tag{12}$$

with $n = 57$; $r = 0.9990$; $u = 0.17$ kcal/mol
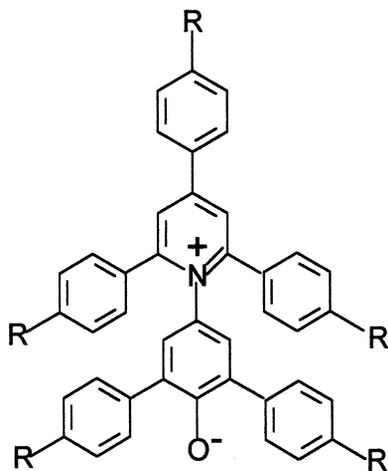
1a, R = H; **1b**, R= t-Bu.

1a,b

Scheme 1

Equation (12) allows the indirect estimation of the $E_T(30)$ values for low polarity solvents.

'Primary' $E_T(30)$ values, that is, those obtained directly from the study of the electronic absorption spectrum of **1a** are generally known within 0.1 kcal/mol. Simple statistical considerations indicate that 'secondary' values, obtained through eqn 12 are affected by an uncertainty of $\sim 2 \times 0.17 = 0.34$ kcal/mol.

The $E_T(30)$ values given in this compilation come from two main sources: (i) Reichardt's 1994 review [3] and (ii) Reichardt & Schäfer's [31a] 1995 paper. The latter contains new data as well as some revised values for selected hygroscopic solvents. We emphasize that the absorption spectra of Dimroth-Reichardt's dyes such as **1a** and **1b** are known to be extremely sensitive to traces of water and other

hydrogen bond donor impurities [32]. Data for super-critical CO_2 are from very recent work by Reichardt and co-workers [31b].

E_T^N is a dimensionless 'normalized' scale, defined through eqn 13:

$$E_T^N(\text{Solvent}) = [E_T(\text{Solvent}) - E_T(\text{TMS})]/[E_T(\text{Water}) - E_T(\text{TMS})] \tag{13}$$

wherein tetramethylsilane (TMS) and water are selected as rather extreme cases of 'polarity'. The values given in this compilation are taken from the same sources as $E_T(30)$.

(Regarding the use of the term *solvatochromism*. According to Reichardt [1]: 'The term solvatochromism is used to describe the pronounced change in position (and sometimes intensity) of an UV-Visible absorption band, accompanying a change in the polarity of the medium...'. This term is widely used. Some experts in the field, notably Kosower, disagree with its use. Thus, he states [16] that: '[solvatochromism]...does not properly reflect the spirit of the probe, which is to probe the microenvironment, be it glass, solid, surface or solvent. I suggest that we change this word to **perichromism**...').

Z (and Z′)

The *Z* scale is due to Kosower [33] and has been widely used. It is based on the high solvent-sensitivity of the frequency of the charge-transfer absorption band of the indicator 1-ethyl-4-carbomethoxypyridinium iodide (**2a**). This band undergoes a substantial bathochromic shift with increasing solvent 'polarity'. The value of *Z* for a given solvent is defined as the molar transition energy (in kcal/mol) for the long wavelength electronic transition of dye **2**, as a solution in this solvent at 25.0 °C and at a pressure of 0.1 MPa. *Z* is also obtained through an expression similar to eqn (11), from the experimentally determined wavelength of the absorption maximum of this transition (λ_{max}).

The values presented in this compilation are mostly taken from Kosower's original publications [33–35] and from the review by Griffiths & Pugh [36] in which values from Pugh's Doctoral Thesis are given [37]. Data from other sources [38–47], are also given. Notice that, in general, data from different origins agree within 0.1 or 0.2 kcal/mol. However, in some cases, particularly in solvents of low polarity, large differences (of up to 5 kcal/mol) are observed. They likely originate in traces of acidic impurities (including water).

Kosower [33] also examined the behavior of the longest wavelength transition in the electronic absorption spectrum of 4-cyano-1-ethylpyridinium iodide (**2b**) (Scheme 2). Medium effects on the corresponding transition energies are linearly related to *Z*-values to a very high degree of correlation [48] and a standard deviation of 0.5 kcal/mol. Marcus [48] suggested the use of the symbol *Z′* for the scale of medium effects based on the solvatochromic shifts undergone by the longest wavelength band in the electronic absorption spectrum of **2b**. We report here the experimental values of *Z′* taken from [45] as well as those given in [48] and determined by means of the correlation between *Z* and *Z′*. For the former, uncertainties are in the range 0.1–0.2 kcal/mol. For the latter, they are estimated in the range 0.5–1 kcal/mol.

2a   **2b**
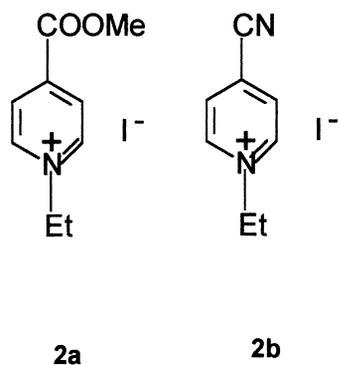
Scheme 2

G and related scales

The *G* scale was developed by Schleyer & Allerhand [49]. It is based on the quantitative study of the solvent shifts undergone by the positions of the *stretching vibrations*, σ, of selected X=O oscillators. These authors defined the *G* scale through eqn (14):

a $G = (\sigma^O - \sigma^S)/\sigma^O$ (14)

wherein σ^O and σ^S, respectively, stand for the positions of the stretching vibration of X=O in the gas phase and in solvent S. a is a constant characteristic of the probe (in [49a], eqn 14 had a misprint, corrected in [49b]). In the actual construction of the scale, these authors used the carbonyl stretching bands of N, N-dimethylformamide and benzophenone [50] and the sulfuryl band of DMSO [51]. These data were taken from the literature and, again, an averaging process was carried out.

Here we report the actual positions of the carbonyl vibrations for the various indicators, labeled σ(CO, I), σ(CO, II) and σ(SO). These data were obtained at 0.1 MPa but the working temperature (likely to be close to 25.0 °C) was not given in the original papers. The stated precision of the σ values is $\pm 1\,cm^{-1}$. Notice that, although the SI unit for σ is m^{-1}, we use cm^{-1} in the Table, as it has been customary in this field. In 1986, Somolinos, García and co-workers [52a] carried out a revision and extension of the *G* scale. These authors also worked at 0.1 MPa at 'room temperature'. The scaling of their data is slightly different from that of [49]. Thus, the value for 1,2-dichloroethane ($G = 95$) was taken as an anchor point instead of that for dichloromethane ($G = 100$), the reason being the definite character of hydrogen bond donor of the latter. We also present these values in Table 2a.

Nicolet, Laurence & Luçon published in 1987 a study on the solvent shifts undergone by the C=O stretching band of methyl trichloroacetate, CCl_3COOMe [53a]. This band has several features that make it particularly suitable as a molecular probe [53a]. Furthermore, as we discuss below, these solvent shifts can be combined with those for trichloroacetic acid, CCl_3COOH, in the same solvents to generate a scale of hydrogen bonding basicities [53a]. The experimental values are taken from [53a]. The positions were determined at 25.0 °C and 0.1 MPa and the stated precision is $0.5\,cm^{-1}$. These values are listed as σ(CO, III).

More recently, Kolling reported the position of the carbonyl stretching vibration of ethyl acetate [52b] and butanone [52c] (at 298.15 K and 0.1 MPa) in a variety of solvents. Uncertainties on these data are given as $\pm 0.5\,cm^{-1}$. These values are presented as σ(CO, IV) and σ(CO, V). Also reported are Notario's [52d] data on the carbonyl stretching band of ethyl acetate in a set of carefully purified solvents at 25.0 °C and 0.1 MPa. The corresponding positions (in cm^{-1}) are listed as (CO, VI) and their uncertainties are estimated at $\pm 1\,cm^{-1}$.

Prof. Laurence [53b] has suggested that in this study, a choice be made among the different IR-based scales. While we acknowledge the fact that at this moment there are 'too many' of them, we feel that the situation is not yet ripe for this choice to be made. There are two main reasons for this: (i) The data sets are fairly limited and it would be necessary to know more about the behavior of the various probes, and (ii) it might well be that the different scales show different sensitivities to the various components of the 'solvent effect'. In particular, there is no proof of the precise equivalence of all rankings of 'polarity' defined by means of these probes. It is to be hoped that this situation prompts further experimental research in the field.

Scales of dipolarity-polarizability

These scales are based on the concept that solvent–solute interactions can be decomposed into 'general' and 'specific' interactions [1]. The former have electrostatic and dispersive origins and can be related (at least conceptually) to reaction field theories. Specific effects include hydrogen-bonding and/or donor–acceptor interactions. The term 'dipolarity' was coined by Kamlet, Abboud & Taft (KAT) [2,54] in order to distinguish the interactions originating essentially in electrostatic effects from the 'overall' interactions included in Reichardt's concept of 'polarity'. It is obvious that this is somehow an oversimplification and that 'multipolar' is certainly more appropriate.

π*

This scale was defined by KAT in 1977 [54]. It was intended to provide a quantitative measure of the

nonspecific part of van der Waals [17a] interactions between solvents and solutes. Operationally, the scale was based on the treatment of the solvatochromic shifts undergone by selected absorption bands of a variety of 'molecular probes'. These probes were aromatic molecules, mostly of the A-C_6H_4-D type (structures **3a** and **3b**), where A and D, respectively, stand for electron-acceptor (such as CN or NO_2) and electron-donor (such as OMe or NEt_2) groups (Scheme 3).

(a) $\bar{D}$——A   (b) $\overset{+}{D}$=—=$\bar{A}$
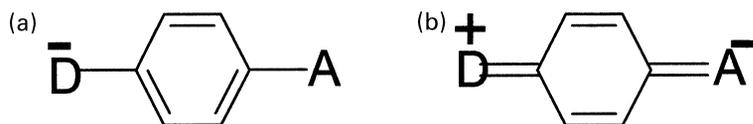
Scheme 3

Experimentally, the following had been found for these compounds: (i) The frequency of the longest wavelength electronic absorption transition is solvent-dependent; (ii) Whenever specific interactions (such as hydrogen bonding) are excluded, medium effects on the frequencies of the solvatochromic bands of any two indicators are linearly related to a high degree of precision. Thus, consider two indicators, for example 1 and 2, and let $\sigma(1)_{S0}$ and $\sigma(2)_{S0}$ stand for the positions of the maxima of their solvatochromic bands in a given reference solvent, $\sigma(1)_S$ and $\sigma(2)_S$ being the corresponding values in solvent S under scrutiny, eqn 15 was found to hold:

$$\sigma(2)_S - \sigma(2)S0 = s[\sigma(1)_S - \sigma(1)_{S0}] \tag{15}$$

where s is a constant dependent solely on 1 and 2.

Given a solvatochromic indicator, the π^* value for a solvent S was defined through eqn 16:

$$\pi^*(S) = [\sigma(S) - \sigma(c\text{-}C_6H_{12})]/[\sigma(DMSO) - \sigma(c\text{-}C_6H_{12})] \tag{16}$$

where the $\sigma(S)$ pertain to the frequencies of the maximum of the solvatochromic band in the various solvents. c-C_6H_{12} (cyclohexane) and DMSO (dimethyl sulfoxide) were used as references by taking $\pi^*(c\text{-}C_6H_{12}) = 0$ and $\pi^*(DMSO) = 1$ by definition.

The actual π^* values for 57 nonhydroxylic solvents (but including some weakly hydrogen-bond donors such as chloroform, dichloromethane and nitromethane) were initially reported by KAT [54]. These values were arrived at by simultaneously solving eqns 15 and 16 for seven 'primary' indicators in this set of solvents. This original set of values was later extended by incorporating new data originating in new experimental work by the KAT group and in studies by Bekarek's [55] and Carr's [56] groups. Seven π^* values were estimated by means of correlation eqns between π^* and functions of n and ε_r. A database of 101 π^* values was thus constructed and published in 1983 [57]. This set has been extensively used over the years and is reported here.

In 1986 Laurence & Nicolet [58] published a careful re-examination of temperature and medium effects on the solvatochromic bands of several of the most important indicators used in KAT's original construction of the π^* scale. For our purposes, the following of their findings are particularly relevant: (1) The solvatochromic band of the indicator 4-(diethylamino)-nitrobenzene (**4**) (the single most widely used indicator in the KAT formalism) has a significant vibrational structure leading to a solvent-dependent band shape. (2) π^* values are somewhat solute-dependent. Clearly, the precision of eqn 15 is not as high as initially believed. (3) Furthermore, it was clearly shown that for a given indicator, π^* values are temperature-dependent ('thermosolvatochromism').

In a Thesis presented in 1991, M. T. Dalati [17b] reported the frequencies of the solvatochromic bands of 4-methoxynitrobenzene (**5**) and 4-(dimethylamino)-nitrobenzene (**6**) in 276 solvents at 25.0 °C and 0.1 MPa. **6** was selected because previous studies had shown that its UV-visible spectrum is not appreciably affected by band shape problems. The solvatochromic band of **5** keeps a constant Gauss-Lorentz band shape all the way from the gas phase to the most polar solvents. A substantial part of these data, together with some new values obtained under the same experimental conditions were reported in 1994 [17a]. The corresponding frequencies of the absorption maxima are noted σ_{NMe2} and σ_{OMe}. The π^* values obtained for each of these two indicators (π^*_{NMe2} and π^*_{OMe}) by means of eqn 16 and the conditions $\pi^*(c\text{-}C_6H_{12}) = 0$ and $\pi^*(DMSO) = 1$ are given in this compilation. Experimental uncertainties on the wavelengths of the absorption maxima can be estimated at ≈ 0.2 nm. In some cases,

and because of spectral interferences σ_{OMe} values could not be determined experimentally and the values reported were obtained by interpolation using the corresponding σ_{NMe2} values and the correlation between σ_{NMe2} and σ_{OMe}.

We draw attention to the fact that the π^* scale was obtained as an average of experimental values for several indicators. This averaging process was aimed at smoothing out indicator-dependent structural effects and there is no doubt that averaging over seven different indicators introduces some degree of smoothing. On the other hand, from the standpoint of similarity, averaging blurs the characteristics of the model. Inspection of π^*, π^*_{NMe2} and π^*_{OMe} values shows that they are generally reasonably close but often show significant quantitative differences. The origin of some of these differences has been discussed in [17a]. It is essentially up to the reader to choose between an 'averaged' dipolarity-polarizability effect (that is, to use π^* or an average of π^*_{NMe2} and π^*_{OMe}) or a scale based on a single indicator.

SPP

This scale has been reported by Catalán and co-workers in 1995 [59]. Although it has not yet been used extensively, we include it in this compilation because it provides experimental data for 100 solvents, most of which are nonhydrogen bond donors or, eventually, very weak donors. Operationally, the scale is based on the solvatochromic shifts undergone by the long wavelength absorption maximum of two indicators: 2-(dimethylamino)-7-nitrofluorene (DMANF, **7**) and 2-fluoro-7-nitrofluorene (FNF, **8**). Experimental uncertainties on the wavelengths of the absorption maxima are ≈ 0.2 nm (Scheme 4).

7   **8**
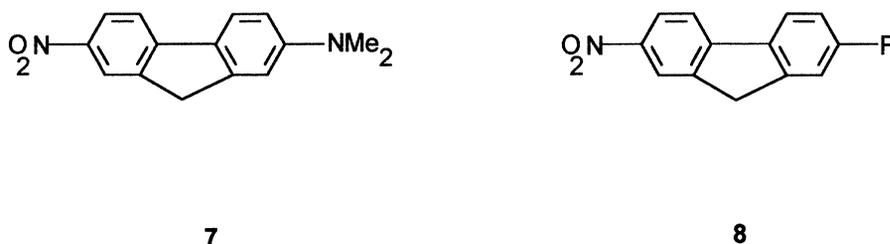
Scheme 4

These indicators are structurally related to those used in the construction of the π^* scale. Their solvatochromic bands are also characterized by substantial bathochromic shifts with increasing dipolarity-polarizability of the solvent. The experimental positions (in cm^{-1}) for the absorption maxima of both indicators, respectively σ_{DMANF} and σ_{FNF} are given in the compilation. Catalán $et\,al.$ assume that band-shape effects are the same for both indicators and that they cancel out in the difference $\Delta\sigma = \sigma_{DMANF} - \sigma_{FNF}$. Accordingly, for a given solvent S, the value of the 'solvent polarity-polarizability' parameter $SPP(S)$ is defined through eqn 17:

$$SPP(S) = [\Delta\sigma(S) - \Delta\sigma(c\text{-}C_6H_{12})]/[\Delta\sigma(DMSO) - \Delta\sigma(c\text{-}C_6H_{12})] \tag{17}$$

This implies the same normalization for both the SPP and the π^* scales.

Catalán $et\,al.$ have set forth a scale with a different normalization (SPP^N) wherein the origin is not $\Delta\sigma(c\text{-}C_6H_{12})$ but rather the calculated value of $\Delta\sigma(gas)$. The scales SPP and SPP^N are given in this compilation. At this point, the only source of data for these scales is [59].

π^*_{azo}

These parameters have been defined by Buncel & Rajagopal [61a]. Operationally, they are based on the solvatochromic shifts undergone by the longest wavelength absorption band ($n{\rightarrow}\pi^*$ and $\pi{\rightarrow}\pi^*$ transitions) of a set of six azo merocyanine dyes (**9–14**) (Schemes 5–7). The position of these maxima is in the region 440–590 nm, far away from the cut-off points of a very large number of solvents. In their study, Buncel & Rajagopal examined the spectra of these indicators in solution in 29 different solvents. Out of these, 25 were either nonhydrogen bond donors or weak hydrogen-bond donors. The frequencies of the maxima were determined at 25.0 °C and under 0.1 MPa and are given in the compilation. The corresponding frequencies σ_{max} (**9**) to σ_{max} (**14**) in the various solvents are linearly related to a very high

degree. That is, for these indicators, eqn 15 holds. Notice that, as in the case of the indicators used by KAT, the standard deviations of these mutual correlations are substantially larger than the experimental uncertainties. The solvatochromic shifts of these indicators were averaged by simultaneously solving eqn 15 for the all of them, as in the case of the construction of the π^* scale. This finally led to the π^*_{azo} scale we report in this compilation. The π^*_{azo} values are also normalized with respect to c-C_6H_{12} and DMSO. It is important to notice that, as shown by Buncel & Rajagopal, the quality of the correlations of medium effects on solute properties obtained using π^* or π^*_{azo} are very close. However, when the solute is an azo compound, π^*_{azo} performs better than π^* and the opposite holds for nitro compounds solutes. It is clear that, notwithstanding the averaging process, all these scales keep some 'model-dependent' specificity, however, small. Detailed discussions on this topic, as well as a general review on the π^*_{azo} scale are given in the 1990 review by Buncel & Rajagopal [61b].
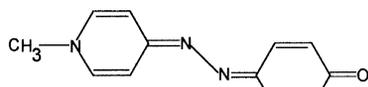
9
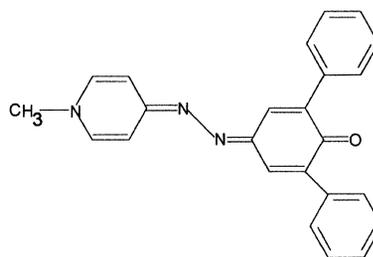
10

Scheme 5
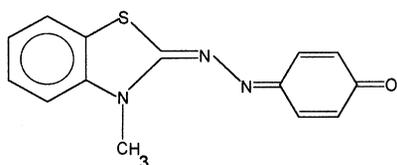
11
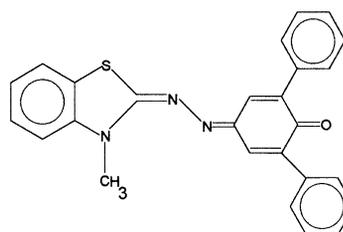
12

Scheme 6

13

14
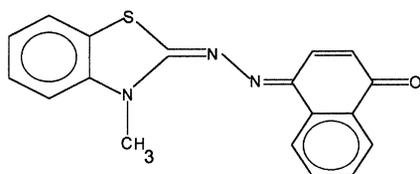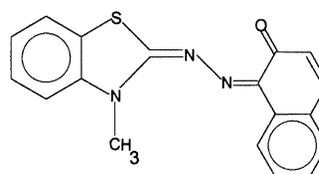
Scheme 7

π^*_2

As indicated earlier, the empirical scales examined above simultaneously reflect two contributions: (1) The electrostatic interactions between the charge distribution of the solute and the permanent or induced dipoles (or higher multipoles) of the solvent and (2) the dispersive solvent–solute interactions. In all these scales, the contribution of the former factor is very important. Thus, they are most suitable for the study of properties of solutes which are also strongly affected by these electrostatic interactions. It is an experimental fact, however, that other properties follow a different pattern of solvent-dependence, largely determined by dispersive interactions. Abe [62] addressed the problem of developing empirical scales suitable for the study of these properties. He developed a scale π^*_2 based on the solvatochromic shifts undergone by the long wavelength electronic absorption transitions of three indicators: naphthalene ($C_{10}H_8$), anthracene ($C_{14}H_{12}$) and β-carotene. The scale was normalized by taking $\pi^*_2 = 0$ for the the gas phase and $\pi^*_2 = 1$ for c-C_6H_{12} solvent. For any given solvent S, $\pi^*_2(S)$ was given by eqn 18:

$$\pi^*_2(S) = [\sigma(S) - \sigma(gas)]/[\sigma(c\text{-}C_6H_{12}) - \sigma(gas)] \tag{18}$$

The frequencies appearing in this equation are for the ^1L_b electronic transition of $C_{10}H_8$ solute. Abe observed that solvent effects on the frequency of the ^1L_a electronic transition of $C_{14}H_{12}$ are linearly related to a high degree of precision. This is a situation similar to that described by eqn 15. This correlation was used to generate π^*_2 values for solvents for which no naphthalene data were available. The frequencies of the absorption maxima of the longest wavelength electronic absorption transition of β-carotene behave analogously and data for this solute were used to further expand the scale and to obtain π^*_2 values for tetrachloromethane and nonane. Abe's original π^*_2 values are given in this compilation. It is important to realize that, through the use of correlations of the form of eqn 15, this scale involves an averaging process. Also, the experimental database includes results obtained in different laboratories. As in the original paper, the π^*_2 values are given in the compilation with three decimal figures but it seems safer to round off to only two, particularly on account of the very small solvent sensitivity of the ^1L_b electronic transition of $C_{10}H_8$ and the built-in averaging process.

The solvatochromic band of β-carotene is in the visible region, far away from the cut-off points of a very large number of solvents. This is a distinct advantage with respect to $C_{10}H_8$ and $C_{14}H_{12}$ indicators. It is also much more sensitive to medium effects than the long wavelength absorption band of these compounds. This has prompted Abe and colleagues [66] to extend the study of the long wavelength absorption band of β-carotene to a wider set of solvents at 25.0 °C and 0.1 MPa. Their results are also presented in the compilation. Uncertainties on the wavelength of the absorption maximum in these solvents can be estimated at ∼0.2–0.3 nm. Notice that the subscript 2 (as in π^*_2) is extensively used for *solute* parameter scales and care must be exercised in order to avoid confusions.

Basicity scales

These scales are intended to quantify the *more specific* solvent–solute interactions in which the solvent plays the role of an electron pair-donor (the solute obviously being an electron pair-acceptor). Such interactions are Lewis-type acid-base (or Lewis-type donor-acceptor) interactions in the classical sense. Other interactions involving some cationic centers have been observed, where the solvent can act as an electron pair donor towards the cation but the cation can also donate d-electrons into the bond to the solvent (π-back donation). Such interactions are called soft–soft interactions.

Here we single out some widely used scales of hydrogen bonding and of 'hard' and 'soft' basicities of solvents. Hydrogen-bonding interactions can be considered as particular cases of 'hard' basicity.

It has been shown [67a] by means of Correlation Analysis techniques that the general, quantitative description of *basicity* requires at least two orthogonal descriptors, F_1 and F_2. It follows that one can envisage an infinite number of 'single parameter' basicity scales (very much as in the case of dipolarity-polarizability). It is an experimental fact, however, that in many cases, the relative weights of the contributions of F_1 and F_2 vary within very narrow limits. This allows the construction of scales of broad applicability.

Hydrogen bonding (HB) basicity scales

'$\Delta\nu_{OD}$' ($\Delta\sigma_{OD}$) and B

The great sensitivity of the O-H (or O-D) oscillators to hydrogen bonding has long been known as it was already used by Stanford and Gordy in 1940 [68] as a tool to quantify the Lewis basicity of molecules. In 1968, Kagiya, Sumida & Inoue [69] determined the positions (in cm^{-1}) of the O-D stretching band of monomeric methan[^{2}H]ol in a variety of solvents. These workers took the difference between the positions of the absorption maximum in solvent S and in benzene, $\Delta\sigma_{OD} = \sigma(S) - \sigma(C_6H_6)$ as a quantitative measure of the HBA character of these solvents. *Notice that in all the studies relevant to this section the notation ν was used for the positions of the bands (in cm^{-1}), instead of σ, the notation presently recommended by the IUPAC*. The formal concentration of methan[^{2}H]ol in these experiments was 0.4 mol/L. Measurements were carried out at $18 \pm 3\,°C$ and under a pressure of 0.1 MPa. Uncertainties on the values of the shifts were estimated at $\pm 1\,cm^{-1}$. The accuracy of the positions is probably in the range 2–3 cm^{-1}. We report the experimental values as $\sigma_{OD}(K)$. Several years later, Burden, Collier & Shorter [70] carried out a revision and extension of this study. Working conditions were similar to those used in [69]. Accuracy and reproducibility were deemed to be better than $\pm 1\,cm^{-1}$. The precision of the σ_{OD} values was estimated at 2–3 cm^{-1}. The results of their study is presented as $\sigma_{OD}(S)$. Notice that this study also reports some values remeasured by Kagiya. They have been included in the σ_{OD} (K) list.

Koppel & Palm [13,71] defined a scale of Lewis basicity of solvents, *B*, through eqn (19):

$$B = \sigma_{OD}(gas) - \sigma_{OD}(S) \tag{19}$$

wherein $\sigma_{OD}(gas)$ and $\sigma_{OD}(S)$ stand for the values of σ_{OD} in the gas phase and in solvent S. In the initial study the experimental data were taken from various sources. These values were revised by Shorter and co-workers on the basis of their study quoted above and are presented here as *B*(KP-S). In cases wherein revised values were not available, the original Koppel-Palm values are given.

B'

A few years after the definition of the *B* scale, Koppel & Paju [71] re-defined the scale *B* of solvent Lewis basicity through eqn 20:

$$B = \Delta\sigma_{PhOH}{}^{CCl4} = \sigma_{PhOH}{}^{CCl4} - \sigma_{PhOH\cdots S}{}^{CCl4} \tag{20}$$

$\Delta\sigma_{PhOH}{}^{CCl4}$ stands for the position (in cm^{-1}) of the O-H stretching mode of monomeric phenol in tetrachloromethane solution. $\sigma_{PhOH\cdots S}{}^{CCl4}$ is the position of the O-H stretching mode of phenol within the 1:1 complex with molecule S in tetrachloromethane solution. It is important to observe that, as emphasized by Koppel & Paju, '...representation of the solvent basicity parameters by eqn 20 is equivalent to the introduction of the postulate that base-induced shifts of the stretching frequencies of the X-H band of the [hydrogen bond] donors in infinite dilution in inert media can also characterize the Lewis basicity of the corresponding pure bases as solvents'. This is an important caveat to consider in Correlation Analysis treatments of medium effects. For the sake of clarity we use the notation B' to avoid possible confusions with the *B* scale defined by means of eqn 19. In this compilation we report data from [71]. These data actually originate in a variety of sources and are noted B'(K-P). It is quite difficult to assess the uncertainties in these values. On the basis of a comparison with data by Pickering, determined under the same experimental conditions, one can reasonably assume an average uncertainty of $\pm 4\,cm^{-1}$ for these parameters. Data determined in 1984 by Makitra and co-workers [72] have also been included as B'(K-P) values. In his PhD work [73], Pickering carried out a careful study of the IR spectra of 1:1 HB complexes between phenol and a variety of bases. Working temperature and pressure were 25.0 °C and 0.1 MPa. Calibration of the IR spectrometer was routinely performed. In a number of cases, e.g. in complexes involving carbonyl compounds, the observed associated band of hydrogen-bonded phenol is actually the envelope of two bands, corresponding to the interactions with the *n* and π electrons of the carbonyl group. Pickering was able to determine the maxima for each one of the two bands. When the deconvolution procedure was not required, the stated uncertainties are in the range of ± 2 to $\pm 4\,cm^{-1}$. We present the σ_{OH} values determined in this study as $\sigma_{OH}(PS)$ (for Pickering & Shorter). They are taken from [73]. The B' values derived through eqn 20 are given as B'(PS). With some significant exceptions the agreement with B'(K-P) is reasonable (within $\pm 4\,cm^{-1}$).

β scales

They are based on the concept of 'solvatochromic comparison method' (SCM) set forth by Kamlet & Taft [2]. Consider a HB donor (HBD) (e.g. 4-nitrophenol) in solution in a solvent able to act as a HB acceptor (HBA). The overall medium effect on the frequency of the solvatochromic band of the indicator reflects both the 'general' (non-specific) solvent effect and the HB solvent–solute interaction. In order to unravel both contributions use is made of a second indicator, structurally very similar to the former (homomorph) but unable to act as an HBD (e.g. 4-methoxynitrobenzene). It is an experimental fact that the solvatochromic shifts undergone by both indicators on going from the gas phase to a variety of non-HBA solvents (or extremely weak ones) (say saturated hydrocarbons, perfluorinated compounds, etc.) are linearly related to a very high degree of precision. The first fundamental assumption of the SCM is that the same linear relationship holds for the nonspecific part of the solvent effect in the presence of HB. The second is that this contribution is proportional to the value of the π^* parameter for the solvent S under scrutiny.

Consider the positions of the solvatochromic bands of the HBD indicator i, and its homomorph j in solvent S, respectively $\sigma_S(i)$ and $\sigma_S(j)$. Equation 21 holds for non-HB solvents:

$$\sigma_S(i) = a_{ij}\sigma_S(j) + b_{ij} \tag{21}$$

In the case of an HBA solvent, the experimental value of $\sigma_S(i)$ is significantly different from the value predicted by eqn 21. The difference, $\Delta\sigma_S(i) = [\sigma_S(i)]_{experimental} - [\sigma_S(i)]_{eqn\,21}$ was taken as an operational measure of the HBA character of the solvent. In the initial work, the couples 4-nitrophenol(**15**)/4-methoxynitrobenzene(**5**) and 4-nitroaniline/4-(diethylamino)-nitrobenzene were used. The β scale of HB basicity was thus constructed on the basis of the scaled ($\beta = 0$ for c-C_6H_{12} and $\beta = 1$ for HMPA) $\Delta\sigma_S(i)$ values determined for these indicators. The database was further extended once it was realized that these 'solvatochromic betas' correlated to a high degree of precision with the logarithms of the equilibrium constants for the 1:1 HB associations between 4-fluorophenol (pK_{HB} scale) [2] or phenol [2] and a large number of bases in CCl_4 solution. Excellent linear correlations were also found with the limiting ^{19}F NMR shifts of 4-fluorophenol within these complexes (Δ) [2].

The initial set of published β-values was thus averaged over these five different properties [2]. Further extensions of the database were carried out as follows: First, data for a new set of three homomorphic couples were added to the initial set [74]. Later on, the SCM was applied in a somewhat 'looser' way: from the previous studies it was known that the nonspecific part of the solvatochromic shifts of the HBD indicators varied linearly with π^* and, by definition, the HB contribution was taken as proportional to the value of the β parameter. It follows that the positions $\sigma_S(i)$ of indicator i in a HBA solvent S can be expressed through eqn 22 wherein a and b are constants:

$$\sigma_S(i) = \sigma_{c\text{-}C_6H_{12}}(i) + a\pi^* + b\beta \tag{22}$$

Equation 22 was first tested for several HBD indicators using a number of solvents for which both π^* and β values were available and then, applied to calculate new β values for solvents for which only the π^* values were known. All the data obtained in these studies, together with some more values determined by the methods indicated above were published in the 1983 review [57]. They are presented in the compilation under the heading β. An extremely detailed description of the methods used for the determination of these parameters is given in the 1981 review by KAT [2].

The SCM concept behind the determination of the 1983 β values was clearly defined but the averaging process involving several homomorphic couples somewhat blurred the model. The averaging of data determined directly by the SCM with results involving Gibbs energies of formation of 1:1 complexes in inert media, NMR shifts and values obtained through the use of eqn 22 essentially eliminated the model process. This notwithstanding, these β values enjoyed a widespread use and have been proven useful in many cases.

As indicated earlier, in their first study of solvatochromic indicators, Nicolet and Laurence [75] showed that 4-(dimethylamino)-nitrobenzene(**6**) is a better indicator than 4-(diethylamino)-nitrobenzene. Furthermore, in a series of experiments performed on carefully purified and dried solvents at 25.0 °C and 0.1 MPa, they were able to compare the homomorphic couples 4-nitrophenol(**15**)/4-methoxynitroben-zene(**5**) and 4-nitroaniline(**16**)/4-(dimethylamino)-nitrobenzene(**6**). These workers confirmed, under

more stringent experimental conditions, that in the absence of HB interactions, the linear relationship between the positions of the homomorphic indicators (that is, the very basis of the SCM) holds to an extremely high degree of precision. They selected the gas phase, perfluoroalkanes, Me_4Si, alkanes, CCl_4, C_2Cl_4, polyhalogenated benzenes and 1,2-dichloroethane as a reference set of media to which they added the very weak HBA monohalobenzenes and 1,2,3-trichlorobenzene and the very weak HBD CH_2I_2 and $HClC=CCl_2$. The number of data points was extended by using data determined at various temperatures (thermosolvatochromic method). The correlation eqns they obtained were as follows:

$$\sigma(\mathbf{15}) = 1.0434\sigma(\mathbf{5}) - 0.57\,cm^{-1} \tag{23}$$

$n = 74;\ r = 0.9980;\ u = 80\,cm^{-1}$

$$\sigma(\mathbf{16}) = 0.9841\sigma(\mathbf{6}) + 3.49\,cm^{-1} \tag{24}$$

$n = 99;\ r = 0.9969;\ u = 115\,cm^{-1}$

We report in this compilation the values of $\sigma(\mathbf{16})$ and $\sigma(\mathbf{15})$ determined by these workers. Then, by strictly applying the SCM to each homomorphic couple, we determined the β values for all the solvents for which data were available. These results are presented as β_{OH} and β_{NH2} values. Operationally, they were computed as indicated in eqs 25 and 26:

$$\beta_{OH} = -\Delta\sigma(\mathbf{15-5})/(2000\,cm^{-1}) \tag{25}$$
$$\beta_{NH2} = -\Delta\sigma(\mathbf{16-6})/(2759\,cm^{-1}) \tag{26}$$

wherein

$$-\Delta\sigma(\mathbf{15-5}) = [1.0434\sigma(\mathbf{5}) - 0.57] - \sigma(\mathbf{15}) \tag{27}$$
$$-\Delta\sigma(\mathbf{16-6}) = [0.9841\sigma(\mathbf{6}) + 3.49] - \sigma(\mathbf{16}) \tag{28}$$

The values $2000\,cm^{-1}$ and $2759\,cm^{-1}$ in eqns 25 and 26 originate in the choice of hexamethylphosphoramide as a reference value ($\beta = 1$ for this solvent). In this medium, $-\Delta\sigma(\mathbf{15-5}) = 2000\,cm^{-1}$ and $-\Delta\sigma(\mathbf{16-6}) = 2759\,cm^{-1}$.

It is important to emphasize that in the initial studies many more values had been obtained using the couple **16**/4-(diethylamino)-nitrobenzene than **15/5**. The reason for this is that the absorption bands of the former couple are found at longer wavelengths. This situation turned out to be unfortunate for two reasons: (1) The effects of vibronic structure of the solvatochromic band of 4-(diethylamino)-nitrobenzene, already discussed above. (2) Two features of **16** as a HBD: (i) with respect to **15**, it is a much weaker HB acid. Thus, it is possible that in the case of very feebly basic solvents a sizable fraction of **16** remains unassociated [76] and (ii) **16** has two 'acidic' hydrogens. It is known that the strength of the second hydrogen bond is affected by both the acidity of the HBD and the stability of the first hydrogen bond [77]. Even if 4-(diethylamino)-nitrobenzene is replaced by **6**, the latter two effects are unavoidable. In the Nicolet-Laurence work, extremely thin cells were used in order to allow the study of a large number of solvents having cutoff regions in the very near-UV region. This allowed the determination of a very large number of β_{OH} values. Also, the temperature was carefully kept constant at 25.0 °C. This was not the case in the determination of the original set of β values. A direct, stringent comparison of β_{OH} and β_{NH2} was then possible. This comparison showed that, while the HBA rankings defined by these parameters are indeed roughly similar, the linear relationship between β_{OH} and β_{NH2} is family dependent. Family dependence was also found [76] when comparing $-\Delta\sigma(\mathbf{15-5})$ and $-\Delta\sigma(\mathbf{16-6})$ to the other properties included in the averaging processes that led to the construction of the 1983 database [57]. Of course, this detailed information was not available at the time the β scale was constructed. As indicated earlier, at least two factors are needed to describe the 'basic' behavior of solvents. Different HBA scales are likely to involve different 'blends' of these factors and hence originate this family dependence. At this point it is unclear whether the behavior of β_{OH} and β_{NH2} stems from a different blend of factors or is simply a consequence of the low HB acidity of **16** or of its having two acidic hydrogens. In any case, the β scale of choice at this point is β_{OH}. Use of β_{NH2} and the original β should be reduced to a minimum.

SB

This scale was developed by Catalán *et al.* in 1996 [78]. It is based on the application of the SCM to the couple of homomorphs 5-nitroindoline (**17**, NI) and 1-methyl-5-nitroindoline (**18**, MNI). Let $\sigma(\mathbf{17})$ and

$\sigma(\mathbf{18})$ be the positions of the longest wavelength absorption band of **17** and **18** in the UV-visible region. The authors consider the difference $\Delta\sigma = \sigma(\mathbf{17}) - \sigma(\mathbf{18})$ to be a quantitative measure of the HBA character of the solvent. The value of the normalized parameter SB ('solvent basicity') for any given solvent is defined through eqn 29:

$$SB = [\Delta\sigma(\text{solvent}) - \Delta\sigma(\text{gas phase})]/[\Delta\sigma(\text{TMG}) - \Delta\sigma(\text{gas phase})] \tag{29}$$

$\Delta\sigma$(gas phase) was obtained by extrapolation of the $\Delta\sigma$ values for *n*-alkanes. TMG is tetramethylguanidine (the solvent leading to the largest HB basicity effects in their study).

Probes **17** and **18** absorb in a region of the UV-visible range that is, well removed from the cut-off region of most common solvents.

Values of SB for 201 solvents, including a number of HBD materials were determined. The estimated uncertainty on the wavelengths of each of the various experimental absorption maxima was estimated at $\pm 0.2 \, \text{nm}$.

A very important fact is the high degree of similarity between SB and β_{OH}. [78] More precisely, with the only exception of the datum for pyridine, SB and β_{OH} correlate to a very satisfactory degree of precision. This suggests that at least, a significant part of the difference in the HB basicity rankings defined by β_{OH} and β_{NH2} originates in the fact that indicator **16** has two 'acidic' hydrogens. Not enough data are available that allow to rule out some degree of family dependence.

Last we notice that aliphatic and alicyclic hydrocarbons, perfluorohexane and tetrachloromethane, have small but finite SB values, some of which are comparable to that of benzene, for example. This does not imply that this study of indicators **17** and **18** is revealing any HB acceptor character of these materials (although other techniques are able to do so). The situation originates in the definition of $\Delta\sigma$. Thus, for the very same set of not HBA solvents, a direct comparison of $\sigma(\mathbf{17})$ and $\sigma(\mathbf{18})$ leads to eqn 30:

$$\sigma(\mathbf{17}) = 1.027\sigma(\mathbf{18}) + 7.32 \times 10^2 \, \text{cm}^{-1} \tag{30}$$

$n = 22, \, r = 0.9995, \, u = 28 \, \text{cm}^{-1}$

The value of u is quite comparable to the experimental error. If departures of $\sigma(\mathbf{17})$ from the behavior prescribed by eqn 30 are used to quantify HB effects, as in the original SCM, these solvents appear as essentially devoid of HB basicity, in agreement with the behavior of β_{OH} and β_{NH2}.

σ_{CO} and $\Delta\sigma_{CO}$

As indicated above, Nicolet, Laurence & Luçon published in 1987 a study on the solvent shifts undergone by the C=O stretching band of methyl trichloroacetate, CCl_3COOMe and trichloroacetic acid [53], CCl_3COOH. The latter is a strong HBD endowed with important properties: (1) Operationally, the formation of a complex $CCl_3COOH\cdots B$ leads to a significant lowering of the values of the carbonyl stretching frequencies. (2) The dimerization constant of CCl_3COOH is smaller than that of acetic acid. (3) The C_{3v} symmetry of the Cl_3C group precludes the appearance of rotamers in the region of the C=O stretching vibrational range. (4) This compound does not show the Fermi resonance phenomenon usual for carbonyl oscillators. Hence, the C=O stretching band is sharp and symmetrical.

These authors studied the couple CCl_3COOMe/CCl_3COOH in a way formally similar to the SCM, namely the 'IR Comparison Method'. Its foundations are as follows: (1) For solvents which are non-HBA or extremely weak HBA and the gas phase, the positions of the C=O stretching bands of both compounds are linearly related to a high degree of precision, eqn 31:

$$\sigma(CCl_3COOH) = 1.1715\sigma(CCl_3COOMe) - 292.8 \, \text{cm}^{-1} \tag{31}$$

$n = 11, \, r = 0.9993, \, u = 0.26 \, \text{cm}^{-1}$

(2) The HB basicity of a HBA solvent is given by the difference, $\Delta\sigma(CCl_3COOH)$, i.e. between the experimental value of $\sigma(CCl_3COOH)$ and the value calculated by means of eqn 29. We present in this compilation both series of values. They are taken from [53] and were determined at $25.0 \, °C$ and $0.1 \, \text{MPa}$.

Notice that the experimental resolution of the experiments is $\approx 0.5 \, \text{cm}^{-1}$. The standard deviation of fit in eqn 31 is of the order of the experimental uncertainty. This is extremely satisfactory and leads us to hope that if more data become available in the future, $\Delta\sigma(CCl_3COOH)$ may well become one of the choice single parameter scales of HB basicity.

Lewis basicities

These scales are intended to provide quantitative measures of the electron-donor ability of solvents, either as bulk materials or as single molecules involved in 1:1 donor–acceptor interactions.

D_s

This scale was defined by Persson, Sandström & Goggin [79] in 1986. It is based on the shifts undergone by the position of the symmetric Hg-Br stretching vibration in mercuric dibromide, $HgBr_2$, on going from the gas phase to the solvent under scrutiny. It is quantitatively defined through eqn 32:

$$D_s = \sigma_{Hg-Br}(gas) - \sigma_{Hg-Br}(solvent) \tag{32}$$

$HgBr_2$ is a 'soft' Lewis acid.

These values were determined by means of Raman spectroscopy (notice the total symmetry of the vibration). Uncertainties on σ values can be estimated at $\approx 1\,cm^{-1}$. The σ values were determined at a temperature close to 25.0 °C. We report in this compilation the D_s values taken from [79a]. Notice that the $\sigma_{Hg-Br}(solvent)$ scale upon which the scale is based reflects both the 'soft' and 'hard' basicities of the solvent [79b] as well as, in principle, 'general' or reaction field effects. As pointed out by Marcus [79c], fairly high concentrations of $HgBr_2$ (≈ 0.2 M) are needed in these studies, exceeding the solubility of this compound in many useful solvents.

μ_M

This scale was developed by Marcus [80]. It is intended to provide an alternative means for determining the 'softness' of the solvent. Its definition, basic hypotheses and physical meaning are taken directly from Marcus' 1987 paper: 'Since water (W) is a 'hard' solvent, the standard molar Gibbs energy of transfer of ions from a reference solvent to other solvents (S), $\Delta_t G°(W{\rightarrow}S)$, should depend on the softness of these solvents in a different manner for hard or soft ions. Other things being equal, hard ions should prefer water and soft ones the softer ones. Among the 'other things' that should be equal are the charge and the size of the ions, since these properties affect the value of $\Delta_t G°(W{\rightarrow}S)$ greatly'.

Most of the data on this quantity available in the literature pertain to univalent ions, and among these the softest is Ag^+. The size of this ion does not match exactly any hard univalent cation, but it is intermediate between those of Na^+ and K^+. Hence, it is expedient to compare the value of $\Delta_t G°(W{\rightarrow}S)$ for Ag^+ with the mean of $\Delta_t G°(W{\rightarrow}S)$ values for Na^+ and K^+. The result is the basis of the softness scale μ_M (for *malakos*, soft in Greek), defined as follows eqn 33:

$$\mu_M = \{[\tfrac{1}{2}][\Delta_t G°(Na^+, W \rightarrow S) + \Delta_t G°(K^+, W \rightarrow S)] - \Delta_t G°(Ag^+, W \rightarrow S)\}/100 \tag{33}$$

The sign of the expression is chosen so as to make μ_M more positive the softer the solvent S is, and the division by 100 (for values of $\Delta_t G°(W{\rightarrow}S)$ expressed in kJ/mol) serves to bring the values of μ_M to a similar magnitude as other property indices of solvents used in linear solvation energy relationships, i.e. approximately between 0 and 1.'

Notice that in Marcus' original work, the 'softness' parameter was represented by μ. Here we use μ_M in order to avoid any confusion with the modulus of the molecular dipole moment. We present in Table 2d the values of μ_M taken from two papers by this author, [80,81]. They have been carefully checked against a list he kindly provided to us.

As regards the precision of the μ_M values, they were estimated by Marcus at ± 0.03. Of course, this uncertainty is determined by the uncertainty on the experimental values of $\Delta_t G°(W{\rightarrow}S)$.

Notice that, because of the definition of μ_M as a difference of terms, individual contributions from cavity terms are likely to be reduced to a minimum.

SP

In 1988, Gritzner [82a] defined the value of the 'softness parameter' SP for a solvent S on the basis of eqn 34:

$$SP(S) = 25 + |\Delta_t G°(BCN \rightarrow S)| \tag{34}$$

The units of SP are kJ/mol. $|\Delta_t G°(BCN{\rightarrow}S)|$ is the absolute value of the standard Gibbs energy change

pertaining to the transfer of Ag^+ from benzonitrile to solvent S. The addition of 25 kJ/mol and the use of the absolute value of $|\Delta_t G°(BCN{\rightarrow}S)|$ are intended to yield positive values in all cases.

In a study published in 1993 [82b], he reported additional $|\Delta_t G°(BCN{\rightarrow}S)|$ values. He also carried out a careful comparison of the results obtained by means of different experimental methods and established that, in general, they agree within 6 kJ/mol. It is only in a few instances that differences reach 7–9 kJ/mol. This suggests that the average uncertainties on μ_M are probably closer to ± 0.06 (see above). It is important that the definitions of μ_M and SP easily allow the updating and extension of these magnitudes as this fundamental thermodynamic information becomes available. Here we report the actual SP values given in [82a] and [82b].

We also draw attention to the concept set forth by Gritzner [79b] relative to the physical meaning of SP: this parameter is essentially a measure of the interactions between soft acceptor solutes and soft solvents. Such interaction, which requires that both the acceptor solutes and the solvents contribute electron-pairs to the bond should be treated separately. According to this author, 'this type of interaction cannot be accounted for by solvent parameters such as the β- and B-parameters, DN and $\Delta H°_{BF3}$. Interactions of soft or hard solvents with solute acceptors which are not capable of undergoing soft–soft interactions can be described by solvent parameters accounting for the hard Lewis-donor properties of the solvents.

Notice that, in principle, the SP scale also contains contributions from a purely electrostatic interaction between Ag^+ and the solvent.

DN and $\Delta H°_{BF3}$

The scale DN ('donicity scale') was developed in 1966 by Gutmann [83] and has been extensively used since then. It precedes all other 'basicity scales' and has played a seminal role in solution chemistry. It is defined operationally as the negative of the standard enthalpy changes, $\Delta H°_{SbCl5}$ for the formation of the 1:1 adduct between antimony pentachloride and electron pair donor solvents D, both in dilute solution in 1,2-dichloroethane at 25.0 °C and 0.1 MPa, according to reaction 35:

$$D(soln) + SbCl_5(soln) \rightleftarrows D{:}SbCl_5(soln) \tag{35}$$

$\Delta H°_{SbCl5}$ is given by eqn 36:

$$\Delta H°_{SbCl5} = \Delta H_1 - \Delta H_2 \tag{36}$$

wherein ΔH_1 and ΔH_2 are the enthalpy changes under standard conditions for reactions 37 and 38, respectively:

$$D(pure\ liquid) + SbCl_5(soln) \rightleftarrows D{:}SbCl_5(soln) \tag{37}$$

and

$$D(pure\ liquid) \rightleftarrows D(soln) \tag{38}$$

All these data were determined by calorimetric techniques. In particular, ΔH_1 was obtained by dissolving pure D into a solution containing an excess of $SbCl_5$.

The DN scale has been very widely used, particularly in the field of coordination chemistry.

Some significant shortcomings of this scale have been reported. A number of side-reactions, including reactions of basic impurities (notably water) have been described. Major anomalies have been reported for triethylamine and HMPA. Maria & Gal [84] have published an extremely careful critical compilation of the available DN values. Of great relevance are the results by Olofsson and co-workers [85]. They are numerous and seem to be very precise. These data are presented here together with their experimental uncertainties. The 'best' values (according to [84]) from Gutmann's work are also given.

$\Delta H°_{BF3}$ has been defined by Maria & Gal [84] as the standard enthalpy change for reaction [39], the formation of the 1:1 adduct between boron trifluoride and electron pair donor solvents D, both in dilute solution in dichloromethane at 25.0 °C and 0.1 MPa:

$$D(soln) + BF_3(soln) \rightleftarrows D{:}BF_3(soln) \tag{39}$$

The experimental method was discontinuous titration calorimetry. Reference [84] gives a succint description of the experimental method as well as a series of references to more detailed treatments of the

experimental methods. It seems that ΔH°_{BF3} values are somewhat less likely to be affected by the same problems as the *DN* numbers. The values reported in the compilation are taken from [84] and from Maria & Gal's 1990 review [92]. The experimental uncertainties are generally below 1 kJ/mol and are given in each case.

[Regarding the use of these scales: some members of the working party hold the view that, notwithstanding the great historical merits of *DN*, the scale of choice for actual correlation studies is ΔH°_{BF3} and recommend that the use of *DN* be discontinued. Other members put both sets of data on an equal footing of quality and practical usefulness. We feel that we should not enter this discussion. The user is advised to exercise great care when solvents pyridine, triethylamine and hexamethylphosphoric triamide are involved in the data set (see above). We feel that the best course of action is to use both scales and to carefully compare the results from the standpoints of the statistical quality and physical meaning. Needless to remind that these scales are *related but different*].

DN and ΔH°_{BF3} are based on the interactions of dilute solutions of the relevant solvents in 1,2-dichloroethane or dichloromethane with the reference substances $SbCl_5$ and BF_3. The underlying hypothesis involved in their use is the assumption that the quantitative ranking of 'donicity' they define also holds for the same compounds acting as *solvents*.

STATISTICAL SCALES

These scales are in principle *model-independent*. They are constructed by statistically averaging medium effects on the physical properties or reactivity data of a wide number of solutes. Potential limitations are the very choice of the solutes and/or properties and eventually the definition of the 'subsidiary conditions' that link these scales to standard physical/chemical concepts. Of the various scales set forth so far we single out two families, because of their frequent use:

A and B

These scales were defined by Swain and co-workers in 1983 [93]. Their study involved 1080 data for 61 solvents and 77 reactions. They were analyzed according to the bilinear model described by eqn 40:

$$P(S) = aA(S) + bB(S) + c \qquad (40)$$

$P(S)$ is the value taken by property P in solvent S. a, b and c are constants depending only on the solute and the property under consideration. *A* and *B* are, respectively, the anion-solvating ('acity') and the cation-solvating ('basity') tendencies of S. The determination of *A* and *B* values was carried out from the statistical study of the database indicated above together with the following subsidiary conditions: $A = B = 0$ for *n*-heptane, $A = B = 1$ for water, $A = 0$ for HMPA and $B = 0$ for trifluoroacetic acid. The latter conditions are 'critical', in the sense that they involve mechanistic assumptions. The study involved both non-HB donors as well as HB donors. We present the available *A* and *B* values in Table 2d, together with their statistically determined uncertainties. The publication of these scales led to a substantial amount of controversy [1]. It is not appropriate to dwell on it, particularly since Prof. Swain is unfortunately no longer with us. However, we must caution the reader that, although the two scales *A* and *B* were constructed with the condition of being orthogonal, we find that for the solvents included in this study, that is, non-HB donors or very weak HB donors *A* and *B* are very strongly correlated: more precisely, if we take all the available values, *A* and *B* are correlated with a correlation coefficient of 0.72. By excluding six solvents the correlation increases up to 0.93. Under these conditions, it is clear that *A* and *B* fail to comply with the mathematical condition of orthogonality imposed on them and with the putative physical meaning they are supposed to convey.

S'

This scale was introduced by Drago in 1992 [94a]. It is based on the statistical treatment of 30 molecular probes and 31 solvents. The latter were chosen in order to avoid 'specific' solvent–solute interactions. Data were analyzed on the basis of the correlation eqn 41:

$$\Delta\chi = S'P + W \qquad (41)$$

In this expression $\Delta\chi$ stands for the effect of the solvent on the physicochemical property under

consideration. S' stands for Drago's 'universal' descriptor of solvent polarity. P is a solute parameter intended to measure the susceptibility of the solute probe to polarity and W a nonzero intercept at $S' = 0$. The scale was anchored by taking $S' = 3.00$ for DMSO. All the available S' values, as updated in [94c] are presented in Table 2d. The original data are given in [88a–c]. Unless reported otherwise, statistical uncertainties are generally taken as 0.01 on the basis of the reported values. S' essentially quantifies dipolar interactions (dipole-dipole, dipole-induced dipole) and because of the choice of the various probe systems, data for solvents of low dipolarity-polarizability are extremely scarce.

Table 2a

No.	$E_T(30)$[a,b]	E_T^N [a]	Z[b]	Z' [c]	$\sigma(CO,I)$[d]	$\sigma(CO,II)$[d]	$\sigma(SO)$[e]	G[f]	$\sigma(CO,III)$[g]	$\sigma(CO,IV)$[h]	$\sigma(CO,V)$[i]	π^* [j]	π^*_{OMe}[k]	π^*_{NMe2}[l]
gas	27.1	−0.111	–	–	1716	1681	0(0)	1788.2	1788.2	1762.2 (1765.5)	–	−1.10[m]	−1.23	−0.90
1	–	–	–	–	–	–	–	–	1783.3	–	–	−0.40[n]	−0.48	−0.34
2	–	–	–	–	–	–	–	–	–	–	–	−0.39[o]	–	–
3	–	–	–	–	–	–	–	36[p]	–	–	–	−0.41[o]	–	–
4	–	–	–	–	–	–	–	–	–	–	–	–	−0.48	−0.30
5	–	–	–	–	–	–	–	–	–	–	–	–	−0.40	−0.26
6	–	–	–	–	–	–	–	–	–	–	–	–	−0.34	−0.24
7	–	–	–	–	–	–	–	–	–	–	–	−0.33[o]	–	–
8	–	–	–	–	–	–	–	–	1782.9	–	–	−0.36[o]	–	–
9	34.2	0.108	–	–	–	–	–	–	–	–	–	–	0.27	0.32
10	(30.9)	(0.006)	–	–	–	–	–	–	–	–	–	–	−0.15	−0.12
11	(31.0)	(0.009)	–	–	–	–	–	–	1778.8	–	–	–	−0.15	−0.10
12	(31.0)	(0.009)	–	–	1696	1671	1085	44(43)	–	1750.5 (1750.2)	1727.0	−0.08	−0.11	−0.08
13	(31.1)	(0.012)	–	–	–	–	–	–	1778.1	–	–	−0.08	−0.06	−0.07
14	(31.1)	(0.012)	–	–	–	–	–	–	–	–	–	–	–	–
15	–	–	60.1[q,r]	–	–	–	–	–	–	–	–	–	–	–
16	(31.0)	(0.009)	–	–	–	–	–	–	–	–	–	–	–	–
17	(31.0)	(0.009)	–	–	–	–	–	–	–	–	–	–	–	–
19	(31.1)	(0.012)	–	–	–	–	–	–	–	–	–	–	−0.01	0.00
23	(30.9)	(0.006)	60.1[s]	–	1694	1670	1084	49(49)	1777.2	1749.6 (1749.2)	1726.1	0.00	0.00	0.00
27	(32.4)	(0.052)	–	–	–	–	–	–	–	–	–	–	–	–
28	(32.2)	(0.046)	–	–	–	–	–	–	–	–	–	–	–	–
29	–	–	–	–	–	–	–	–	–	–	–	–	0.34	0.32
30	–	–	–	–	–	–	–	–	–	–	–	–	0.37	0.42
31	–	–	–	–	–	–	–	–	–	–	–	–	0.31	0.30
32	–	–	–	–	–	–	–	–	–	–	–	–	0.37	0.41
33	–	–	–	–	–	–	–	–	–	–	–	–	0.30	0.28
34	–	–	–	–	–	–	–	–	–	–	–	–	0.34	0.27
35	(31.2)	(0.015)	–	–	–	–	–	–	–	–	–	–	0.09	0.09
36	–	–	–	–	–	–	–	–	–	–	–	–	0.15	0.17
37	–	–	–	–	–	–	–	–	–	–	–	–	0.21	0.24

Table 2a *Continued*

No.	$E_T(30)^{a,b}$	$E_T^{N\,a}$	Z^b	$Z'^{\,c}$	$\sigma(CO,I)^d$	$\sigma(CO,II)^d$	$\sigma(SO)^e$	G^f	$\sigma(CO,III)^g$	$\sigma(CO,IV)^h$	$\sigma(CO,V)^i$	$\pi^{*\,j}$	$\pi^*_{OMe}{}^k$	$\pi^*_{NMe2}{}^l$
38	(30.7)	(0.000)	–	–	–	–	–	–	–	–	–	–	−0.12	−0.08
39	34.3	0.111	54.0^t	54.0	1684	1663	1068	80(79)	1771.7	1740.2 (1740.0)	1719.0	0.59	0.55	0.59
40	33.9	0.099	–	–	1686	1665	1070	74(75)	–	1739.5 (1739.5)	1717.7	0.54	0.49	0.49
42	–	–	–	–	–	–	–	(73)	–	(1742.5)	–	0.47	–	–
43	33.1	0.074	–	–	–	–	–	–	1773.1	–	–	0.43	0.45	0.41
44	(32.9)	(0.068)	–	–	–	–	–	–	–	1742.3	–	0.41	0.45	0.38
45	(33.0)	(0.071)	–	–	–	–	–	–	1773.3	–	–	–	0.45	0.42
47	–	–	–	–	–	–	–	–	–	–	–	0.41	–	–
48	34.2	0.108	–	–	–	–	–	–	–	–	–	–	–	–
49	–	–	–	–	–	–	–	–	–	–	–	–	0.69	0.67
50	(35.3)	(0.142)	–	–	–	–	–	–	–	–	–	–	0.78	0.80
51	33.5	0.086	–	–	–	–	–	–	–	–	–	–	–	–
52	32.4	0.052	–	–	1687	1667	1071	69(72)	1774.4	1742.4^u (1742.2)	1721.0	0.28	0.21	0.24
53	(33.3) (20 °C)	(0.080) (20 °C)	–	–	–	–	–	–	–	–	–	–	0.10	0.18
54	(34.8)	(0.126)	–	–	–	–	–	–	–	–	–	–	0.41	0.38
55	39.4	0.269	62.1^v	58.3	–	–	–	–	–	–	–	–	–	–
56	41.3	0.327	63.4^v	–	1677	1660	1061	95(95)	–	1735.0 (1735.0)	–	0.81	0.73	0.77
57	36.2	0.170	–	–	–	–	–	–	–	1735.4	–	0.49	0.44	0.51
58	40.3	0.296	–	–	–	–	–	–	–	–	–	–	0.78	0.78
59	(33.8)	(0.096)	–	–	–	–	–	–	–	–	–	–	0.01	0.12
60	(33.2)	(0.077)	–	–	–	–	–	–	–	–	–	–	0.02	0.13
61	37.0	0.194	–	–	–	–	–	–	–	–	–	–	–	–
62	(41.9)	(0.346)	63.9^w	–	–	–	–	–	–	–	–	–	0.72	0.77
63	(34.2)	(0.108)	–	–	–	–	–	–	–	–	–	0.44	0.33	0.33
64	35.9	0.160	–	–	–	–	–	–	–	–	–	0.53	0.48	0.52
65	(32.1)	(0.043)	–	–	1689	1667	1074	64(65)	1774.7	1744.1 (1744.0)	1721.2	0.28	0.25	0.25
66	37.4	0.207	–	–	–	–	–	–	–	–	–	–	0.43	0.50
67	40.2	0.293	–	–	–	–	–	–	–	–	–	–	–	–

68	37.9	0.222	–	–	–	–	–	–	–	–	–	–	–	0.46	0.56
69	40.7	0.309	–	–	–	–	–	–	–	–	–	–	–	–	–
70	(33.6)	(0.089)	–	–	–	–	–	–	–	–	–	–	–	−0.12	−0.03
71	40.4	0.299	–	–	–	–	–	–	–	–	–	–	–	0.78	0.79
72	(32.8)	(0.065)	–	–	–	–	–	–	–	–	–	–	–	0.39	0.34
73	–	–	–	–	–	–	–	–	–	–	–	–	0.39	0.40	0.46
74	39.5	0.272	–	–	–	–	–	–	–	–	–	–	–	0.66	0.71
75	(32.2)	(0.046)	–	–	–	–	–	–	–	–	–	–	–	0.23	0.28
76	(33.3)	(0.080)	–	–	–	–	–	–	–	–	–	–	–	−0.05	0.04
77	(32.8)	(0.065)	–	–	–	–	–	–	–	–	–	–	–	–	–
78	36.2	0.170	–	–	–	–	–	–	–	–	–	–	–	–	–
79	(36.6)	(0.182)	–	–	–	–	–	–	–	–	–	–	–	0.52	0.60
81	37.6	0.213	–	–	–	–	–	–	–	–	–	–	–	0.53	0.61
82	38.3	0.235	60.0[x]	–	–	–	–	–	–	–	–	–	0.75	–	–
83	–	–	–	–	–	–	–	–	–	–	–	–	–	0.49	0.57
84	–	–	–	–	–	–	–	–	–	–	–	–	–	0.47	0.52
85	–	–	–	–	1678	1662	1064	89	–	–	–	–	–	0.73	0.72
86	36.5	0.179	–	–	1667	1655	1050	–	–	–	–	–	1.12[n]	1.00	1.01
87	–	–	–	–	–	–	–	–	–	–	–	–	–	0.65	0.66
88	–	–	–	–	–	–	–	–	–	–	–	–	–	0.60	0.63
90	–	–	–	–	–	–	–	–	–	–	–	–	–	0.53	0.57
91	37.0	0.194	–	–	–	–	–	–	–	–	–	–	0.62	0.59	0.65
92	39.3	0.265	–	–	–	–	–	–	–	–	–	–	–	0.72	0.69
93	37.3	0.204	–	–	–	–	–	–	–	–	–	–	–	0.50	0.59
94	36.4	0.176	–	–	–	–	–	–	–	–	–	–	–	0.49	0.57
95	(33.2)	(0.077)	–	–	–	–	–	–	–	–	–	–	–	0.18	0.24
96	(38.5)	(0.241)	–	–	–	–	–	–	–	–	–	–	–	0.50	0.60
97	–	–	–	–	–	–	–	–	–	–	–	–	–	0.34	0.41
98	36.8	0.188	58.0[w]	–	–	–	–	(84)	–	(1733.0)	–	0.71	0.68	0.69
99	38.0	0.225	60.0[w]	–	–	–	–	(88)	1770.9	(1737.0)	–	0.80	0.77	0.76
100	36.7	0.185	–	–	–	–	–	–	–	–	–	0.67	0.65	0.66
101	–	–	–	–	–	–	–	–	–	–	–	–	0.43	0.48
102	–	–	–	–	–	–	–	–	–	–	–	–	0.65	0.68
103	36.2	0.170	–	–	–	–	–	–	–	–	–	–	0.66	0.66
104	–	–	–	–	–	–	–	–	–	–	–	–	0.67	0.70
105	37.0	0.194	–	–	–	–	–	–	–	–	–	–	–	–
106	36.6	0.182	59.2[w]	–	–	–	–	(88)	–	(1734.5)	–	0.79	0.77	0.72
107	37.6	0.213	–	–	–	–	–	–	1769.6	–	–	–	0.90	0.82

Table 2a *Continued*

No.	$E_T(30)^{a,b}$	$E_T^{N\ a}$	Z^b	$Z'^{\ c}$	$\sigma(CO,I)^d$	$\sigma(CO,II)^d$	$\sigma(SO)^e$	G^f	$\sigma(CO,III)^g$	$\sigma(CO,IV)^h$	$\sigma(CO,V)^i$	$\pi^{*\ j}$	$\pi^*_{OMe}{}^k$	$\pi^*_{NMe2}{}^l$
108	36.5	0.179	–	–	–	–	–	–	–	–	–	–	0.77	0.73
109	(34.7)	(0.123)	–	–	–	–	–	–	–	–	–	–	0.62	0.67
110	36.2	0.170	–	–	–	–	–	–	–	–	–	0.81	0.84	0.78
111	36.9	0.191	–	–	–	–	–	–	–	–	–	–	1.01	1.02
112	45.6	0.460	71.3^q	–	1676	1662	1061	93(94)	1770.5	1736.5 (1736.0)	1714.1	0.75	0.66	0.78
113	43.6	0.398	–	–	–	–	–	–	–	–	–	0.71	0.64	0.74
114	42.5	0.364	67.8^x	–	–	–	–	–	–	1736.7^u	1714.4	0.71	0.63	0.73
115	42.4^y	0.361^y	63.2^x	–	–	–	–	–	–	–	–	–	0.63	0.72
116	–	–	–	–	–	–	–	–	–	–	–	–	0.63	0.70
117	–	–	–	–	–	–	–	–	–	–	–	–	0.58	0.65
118	–	–	–	–	–	–	–	–	–	–	–	–	0.58	0.63
119	–	–	–	–	–	–	–	–	1767.2	–	–	–	0.93	1.00
120	40.0	0.287	–	–	–	–	–	–	–	–	–	–	0.58	0.65
121	–	–	–	–	–	–	–	–	–	–	–	–	0.55	0.68
122	44.4	0.423	–	–	–	–	–	–	–	–	–	–	–	–
123	46.7	0.494	–	–	–	–	–	–	–	–	–	–	–	–
124	41.5	0.333	65.0^w	60.6	–	–	–	(94)	–	1736.0^u (1736.0)	1714.0	0.90	0.88	0.84
125	42.7	0.370	–	–	–	–	–	–	–	–	–	0.99	0.93	0.98
126	43.8	0.404	–	–	–	–	–	–	1769.7	–	–	–	0.75	0.82
127	43.3	0.389	–	–	–	–	–	–	–	–	–	–	–	–
128	42.0	0.349	–	–	–	–	–	–	–	–	–	–	–	–
129	34.5	0.117	–	–	1688	1668	–	64(64)	1775.0	1743.5	1721.2	0.27	0.24	0.31
130	34.0	0.102	–	–	–	–	–	–	–	–	–	(0.27)	–	–
131	(34.1)	(0.105)	–	–	–	–	–	(61)	–	1744.6	1721.6	0.27	0.19	0.26
132	(33.0)	(0.071)	60.1^z 64.0^x	–	1690	1668	1076	61(59)	1775.5	1745.2	1722.1	0.24	0.18	0.24
133	–	–	–	–	–	–	–	–	–	–	–	–	0.13	0.18
134	35.3 (30 °C)	0.142 (30 °C)	–	–	–	–	–	(86)	–	(1737.9)	–	0.66	–	–
135	36.3	0.173	–	–	–	–	–	–	–	–	–	0.80	0.80	0.76
137	34.7	0.124	–	–	–	–	–	–	–	–	–	–	–	–
138	33.7^{aa}	0.093^{aa}	–	–	–	–	–	–	–	–	–	–	–	–

139	(34.4)	(0.114)	–	–	–	–	–	–	–	–	–	–	–	–
140	36.2	0.170	–	–	–	–	–	–	–	–	–	–	–	–
141	37.1	0.198	–	–	–	–	–	(88)	–	(1736.5)	–	0.73	0.70	0.72
142	36.6	0.182	58.9[bb]	–	–	–	–	–	–	–	–	(0.69)	0.65	0.69
143	–	–	–	–	–	–	–	–	–	–	–	–	0.36	0.36
144	41.6	0.336	–	–	–	–	–	–	–	–	–	–	0.77	0.80
145	35.8	0.157	–	–	–	–	–	–	–	–	–	–	–	–
146	33.9	0.099	–	–	–	–	–	–	–	–	–	–	–	–
147	38.2	0.231	59.1[cc] 61.2[dd]	–	–	–	–	–	–	–	–	0.53	–	–
148	38.6	0.244	–	–	–	–	–	–	–	–	–	0.64	–	–
149	38.9	0.253	61.3[bb]	–	–	–	–	–	–	–	–	–	–	–
150	37.5	0.210	65.2[z]	–	–	–	–	–	–	–	–	–	–	–
151	38.4	0.238	–	–	–	–	–	–	–	–	–	–	–	–
152	–	–	–	–	–	–	–	–	–	–	–	0.58	–	–
153	–	–	–	–	–	–	–	–	–	–	–	0.35	–	–
154	(36.0)	(0.164)	–	–	–	–	–	–	–	–	–	–	0.48	0.54
155	37.4	0.207	58.8[bb] 64.0[ee]	56.0	–	–	–	(78)	–	1739.0 (1741.4)	1716.2	0.58	0.55	0.63
156	36.5	0.179	55.3[cc]	–	–	–	–	–	–	–	–	–	–	–
157	35.1	0.136	–	–	–	–	–	–	–	–	–	–	0.39	0.40
158	–	–	–	–	–	–	–	–	–	–	–	–	0.26	0.32
159	36.2	0.170	–	–	–	–	–	–	–	1739.8[u]	1717.6	0.51	0.48	0.52
160	35.5	0.148	–	–	–	–	–	–	–	–	–	–	–	–
161	36.0	0.164	64.6[x]	61.1	1680	1663	–	86	1770.7	–	–	0.55	0.49	0.57
162	43.1	0.383	–	–	–	–	–	–	–	–	–	–	0.63	0.70
163	41.5	0.333	–	–	–	–	–	–	–	–	–	–	–	–
164	44.5	0.426	–	–	–	–	–	–	–	–	–	–	–	–
165	39.8	0.281	–	–	–	–	–	–	–	–	–	–	–	–
166	44.5	0.426	–	–	–	–	–	–	–	–	–	–	–	–
167	42.2	0.355	65.5[cc] 65.7[q]	61.8	–	–	–	–	–	1737.0	–	0.71	0.62	0.71
168	41.3	0.327	64.0[x]	60.4	–	–	–	(85)	–	1737.1	1717.1	0.67	0.60	0.70
169	40.9	0.315	62.0[ff]	58.3[gg]	–	–	–	–	–	–	–	–	–	–
170	39.0	0.256	–	–	–	–	–	–	–	–	–	–	–	–
171	41.1	0.321	63.3[x]	–	–	–	–	–	–	–	–	–	–	–
172	39.3	0.265	–	–	–	–	–	–	–	–	–	(0.72)	0.57	0.67
173	39.4	0.269	–	–	–	–	–	–	–	–	–	–	–	–

Table 2a *Continued*

No.	$E_T(30)^{a,b}$	$E_T^{N\,a}$	Z^b	$Z'^{\,c}$	$\sigma(CO,I)^d$	$\sigma(CO,II)^d$	$\sigma(SO)^e$	G^f	$\sigma(CO,III)^g$	$\sigma(CO,IV)^h$	$\sigma(CO,V)^i$	$\pi^{*\,j}$	$\pi^*_{OMe}{}^k$	$\pi^*_{NMe2}{}^l$
174	38.7	0.247	–	–	–	–	–	–	–	–	–	–	0.58	0.61
176	40.1	0.290	–	–	–	–	–	–	–	–	–	–	–	–
177	38.9	0.253	–	–	–	–	–	–	–	–	–	–	–	–
178	38.0	0.225	–	–	–	–	–	–	–	–	–	–	–	–
179	37.5	0.210	–	–	–	–	–	–	–	–	–	–	–	–
180	39.4	0.269	–	–	–	–	–	–	–	–	–	0.76	0.71	0.76
181	39.8	0.281	–	–	–	–	–	–	–	–	–	0.76	0.68	0.75
182	–	–	65.4^q	–	–	–	–	–	–	–	–	0.66	–	–
183	–	–	–	–	–	–	–	–	–	–	–	0.63	–	–
184	40.6	0.306	–	–	–	–	–	–	–	(1743.5)	–	0.90	0.81	0.48
185	49.2	0.571	–	–	–	–	–	–	–	–	–	–	–	–
186	45.9	0.469	–	–	–	–	–	–	–	–	–	–	0.63	0.70
187	–	–	–	–	–	–	–	–	–	–	–	–	0.49	0.48
188	–	–	–	–	–	–	–	–	–	–	–	–	0.77	–
189	41.9	0.346	70.3^{ff}	66.6	–	–	–	–	–	–	–	0.62	0.55	0.59
190	38.9	0.253	–	–	–	–	–	–	–	–	–	0.60	0.49	0.60
191	–	–	–	–	–	–	–	–	–	–	–	–	0.48	0.52
192	–	–	–	–	–	–	–	–	–	–	–	–	0.44	0.49
193	–	–	–	–	–	–	–	–	–	–	–	–	0.43	0.45
194	–	–	–	–	–	–	–	–	–	–	–	–	0.43	0.45
195	–	–	–	–	–	–	–	–	–	–	–	–	0.40	0.42
196	–	–	–	–	–	–	–	–	–	–	–	–	0.38	0.39
197	–	–	–	–	–	–	–	–	–	–	–	–	0.37	0.39
198	–	–	–	–	–	–	–	–	–	–	–	–	0.43	0.48
199	–	–	–	–	–	–	–	–	–	–	–	–	0.36	0.38
200	38.8	0.250	–	–	–	–	–	–	–	–	–	–	–	–
201	37.9	0.222	–	–	–	–	–	–	–	–	–	–	–	–
203	–	–	–	–	–	–	–	–	–	–	–	0.39	0.36	0.55
204	39.6	0.275	–	–	–	–	–	–	–	–	–	–	0.61	0.67
205	40.9	0.315	–	–	–	–	–	–	–	1738.2	–	0.61	–	–
206	38.1	0.228	59.4^v 64.0^x	58.7	–	–	–	–	–	1740.1	1717.0	0.55	0.45	0.56
207	49.4	0.577	–	–	–	–	–	–	–	–	–	0.61	–	–
208	51.1	0.630	–	–	–	–	–	–	–	–	–	–	–	–

209	38.1	0.228	–	–	–	–	–	–	–	–	–	0.74	0.68	0.71
210	39.4	0.269	–	–	–	–	–	–	–	–	–	0.70	0.67	0.72
211	38.7	0.247	–	–	–	–	–	–	–	–	–	0.61	0.56	0.63
213	37.5	0.210	–	–	–	–	–	–	–	–	–	–	–	–
214	38.5	0.241	–	–	–	–	–	–	–	1741.2	–	0.46	–	–
216	38.0	0.225	–	–	–	–	–	–	–	–	–	–	–	–
217	38.2	0.232	64.7[x]	–	–	–	–	–	–	–	–	–	0.47	0.57
218	36.7	0.185	64.6[x]	–	–	–	–	–	–	–	–	0.45	0.40	0.46
219	–	–	–	–	–	–	–	–	–	–	–	0.64	–	–
220	48.6 (40 °C)	0.552 (40 °C)	–	–	–	–	–	–	–	–	–	–	–	–
221	–	–	–	–	–	–	–	–	–	–	–	–	0.92	1.00
222	46.0	0.472	72.4[z]	–	–	–	–	–	–	–	–	0.83	0.83	0.89
223	44.3	0.420	–	–	–	–	–	–	–	–	–	0.87	0.85	0.91
224	–	–	–	–	–	–	–	–	–	–	–	–	0.89	0.91
225	(43.9)	(0.407)	–	–	–	–	–	–	–	–	–	0.76	–	–
226	–	–	–	–	–	–	–	–	–	–	–	–	0.69	0.72
227	40.4	0.299	–	–	–	–	–	–	–	–	–	–	0.63	0.66
228	–	–	–	–	–	–	–	–	–	–	–	–	0.39	0.44
229	40.7	0.309	–	–	–	–	–	–	–	–	–	–	–	–
230	39.5	0.272	–	–	–	–	–	–	–	–	–	–	–	–
231	43.2	0.386	68.4[cc] 68.5[q]	65.3	–	–	–	–	–	1733.7	1712.1	0.88	0.88	0.87
232	42.9	0.377	66.9[hh]	–	–	–	–	–	–	1732.9	1711.5	0.88	0.85	0.85
233	–	–	–	–	–	–	–	–	–	–	–	–	0.80	0.81
234	–	–	–	–	–	–	–	–	–	–	–	–	0.80	0.80
235	41.4	0.330	–	–	–	–	–	–	–	–	–	–	0.85	0.79
236	44.0	0.410	–	–	–	–	–	–	–	–	–	–	–	–
237	40.8	0.312	–	–	–	–	–	–	–	–	–	–	0.93	0.93
238	40.9	0.315	–	–	–	–	–	–	–	–	–	0.83	0.79	0.80
239	–	–	–	–	–	–	–	–	–	–	–	–	0.66	0.69
240	–	–	–	–	–	–	–	–	–	–	–	–	0.90	0.86
241	42.1	0.352	–	–	–	–	–	–	–	–	–	(1.08)[ii]	–	–
242	42.2	0.355	–	–	–	–	–	–	–	1732.8	1711.4	0.92	0.92	0.90
243	42.8	0.373	–	–	–	–	–	–	–	–	–	–	–	–
244	41.6	0.336	–	–	–	–	–	–	–	–	–	–	–	–
245	40.4	0.299	–	–	–	–	–	–	–	–	–	–	–	–
246	41.6	0.336	–	–	–	–	–	–	–	–	–	–	–	–

Table 2a *Continued*

No.	$E_T(30)^{a,b}$	$E_T^{N\ a}$	Z^b	$Z'^{\ c}$	$\sigma(CO,I)^d$	$\sigma(CO,II)^d$	$\sigma(SO)^e$	G^f	$\sigma(CO,III)^g$	$\sigma(CO,IV)^h$	$\sigma(CO,V)^i$	$\pi^{*\ j}$	$\pi^*_{OMe}{}^k$	$\pi^*_{NMe2}{}^l$
247	42.6	0.367	–	–	–	–	–	–	–	–	–	–	–	–
248	42.1	0.352	–	–	–	–	–	–	–	–	–	–	–	–
249	42.8	0.373	–	–	–	–	–	–	–	–	–	–	–	–
250	43.6	0.398	70.4^x	–	–	–	–	–	1769.1	–	–	–	0.73	0.81
251	41.7	0.324	64.5^x	–	–	–	–	–	–	–	–	0.72	0.69	0.75
252	40.5	0.302	–	–	–	–	–	–	–	–	–	–	–	–
253	38.9	0.253	61.3^x	–	–	–	–	–	–	–	–	0.65	0.63	0.67
254	–	–	–	–	–	–	–	–	1770.9	–	–	–	0.66	0.74
255	40.9	0.315	62.8^{jj}	–	–	–	–	–	–	–	–	0.87	0.87	0.85
256	39.5	0.272	–	–	–	–	–	–	–	–	–	–	–	–
257	42.3	0.358	–	–	–	–	–	–	–	–	–	–	–	–
258	–	–	–	–	–	–	–	–	–	–	–	–	0.70	0.80
259	–	–	–	–	–	–	–	–	–	–	–	–	0.73	0.76
260	–	–	–	–	–	–	–	–	1771.6	–	–	–	0.62	0.71
261	45.1	0.444	70.2^x 71.1^q	67.0	–	–	–	–	–	1731.3 (1732.5)	1710.6	1.00	1.00	1.00
262	–	–	–	–	–	–	–	–	–	–	–	–	1.03	1.00
263	44.0	0.410	70.6^x 77.5^{hh}	–	–	–	–	–	–	1731.8^u	1710.8	0.98	0.90	0.97
264	44.0	0.410	–	–	–	–	–	–	–	–	–	–	–	–
265	43.0	0.380	–	–	–	–	–	–	–	–	–	–	–	–
266	41.0	0.318	–	–	–	–	–	–	–	–	–	–	–	–
267	40.5	0.302	64.0^q	60.3	1677	1661	–	94	–	1736.2^u	1714.0	0.87	0.87	0.84
268	38.3	0.235	–	–	–	–	–	–	–	–	–	–	–	–
269	39.5	0.272	–	–	–	–	–	–	–	–	–	(0.84)	0.80	0.80
270	36.9	0.191	–	–	–	–	–	–	–	–	–	(0.80)	0.67	0.68
271	38.9	0.253	–	–	–	–	–	–	–	–	–	–	0.81	0.79
272	36.4	0.176	–	–	–	–	–	–	–	–	–	–	0.66	0.67
273	(34.0)	(0.102)	–	–	–	–	–	–	–	–	–	–	0.30	0.32
274	44.2 (30 °C)	0.417 (30 °C)	–	–	–	–	–	–	–	–	–	–	–	–
275	42.4	0.361	–	–	–	–	–	–	1770.2	–	–	–	0.79	0.82
276	43.3	0.389	–	–	–	–	–	–	1771.2	–	–	–	0.75	0.78
277	36.3	0.173	–	–	–	–	–	–	1770.7	–	–	–	0.44	0.53

278	41.9	0.346	–	–	–	–	–	–	–	–	–	–	–	–
279	–	–	–	–	–	–	–	–	–	–	–	–	0.98	0.93
280	39.7	0.278	–	–	–	–	–	–	–	–	–	–	0.90	0.82
281	–	–	–	–	–	–	–	–	–	–	–	–	0.86	0.88
282	39.4	0.269	–	–	–	–	–	–	–	–	–	(0.92)	0.93	0.95
283	(32.1)	(0.043)	–	–	1690	1668	–	62(59)	–	(1747.0)	–	0.14	0.09	0.18
284	(32.1)	(0.043)	–	–	–	–	–	(54)	–	(1747.0)	–	0.16	0.06	0.12
285	–	–	–	–	–	–	–	–	–	–	–	–	0.23	0.28
286	–	–	–	–	–	–	–	–	–	–	–	0.49	0.47	0.43
287	36.5	0.179	–	–	–	–	–	(88)	–	–	–	0.90	0.76	0.78
288	–	–	–	–	–	–	–	–	–	–	–	–	0.20	0.24
290	–	–	–	–	–	–	–	–	–	–	–	–	0.30	0.34
291	–	–	–	–	–	–	–	–	–	1772.0	–	–	0.50	0.60
292	–	–	–	–	–	–	–	–	–	1773.1	–	–	0.44	0.47
293	–	–	–	–	–	–	–	–	–	1774.2	–	–	0.35	0.39
294	–	–	–	–	–	–	–	–	–	1773.8	–	–	0.34	0.37
295	–	–	–	–	–	–	–	–	–	1774.8	–	–	–	–
296	–	–	–	–	–	–	–	–	–	1770.5	–	–	0.68	0.71
297	–	–	–	–	–	–	–	–	–	1772.1	–	–	0.61	0.64
298	–	–	–	–	–	–	–	–	–	–	–	–	0.68	0.71
299	35.4	0.145	–	–	–	–	–	–	–	–	–	–	0.67	0.68
300	36.7	0.185	–	–	–	–	–	–	–	1770.9	–	–	0.60	0.68
301	–	–	–	–	–	–	–	–	–	–	–	–	0.55	0.63
302	37.0	0.194	–	–	–	–	–	–	–	1769.5	–	0.16	–	0.78
303	46.3	0.481	71.2[bb]	68.2	1675	1660	–	99	–	1732.2[u]	1711.0	0.85	0.75	0.88
304	43.6	0.398	–	–	–	–	–	–	–	–	–	–	0.77	0.79
305	–	–	–	–	–	–	–	–	–	–	–	–	0.66	0.73
306	–	–	–	–	–	–	–	–	–	–	–	–	0.60	0.69
307	39.6	0.275	–	–	–	–	–	–	–	–	–	–	–	–
308	41.2	0.324	–	–	–	–	–	–	–	1736.3[u]	1714.4	1.01	0.86	0.88
309	–	–	–	–	–	–	–	–	–	–	–	–	0.48	0.53
310	(36.5)	(0.179)	–	–	–	–	–	–	–	–	–	–	0.38	0.41
311	–	–	–	–	–	–	–	–	–	–	–	–	0.59	0.65
312	–	–	–	–	–	–	–	–	–	–	–	–	0.73	0.75
313	35.4	0.145	–	–	–	–	–	–	–	–	–	–	0.35	0.37
314	–	–	–	–	–	–	–	–	–	–	–	–	0.20	0.26
315	–	–	–	–	–	–	–	–	–	–	–	–	0.43	0.44
316	–	–	–	–	–	–	–	–	–	–	–	–	0.54	0.57

Table 2a *Continued*

No.	$E_T(30)^{a,b}$	$E_T^{N\,a}$	Z^b	$Z'^{\,c}$	$\sigma(CO,I)^d$	$\sigma(CO,II)^d$	$\sigma(SO)^e$	G^f	$\sigma(CO,III)^g$	$\sigma(CO,IV)^h$	$\sigma(CO,V)^i$	$\pi^{*\,j}$	$\pi^*_{OMe}{}^k$	$\pi^*_{NMe2}{}^l$
317	–	–	–	–	–	–	–	–	–	–	–	–	0.36	0.37
318	35.	0.148	–	–	–	–	–	–	–	–	–	–	0.50	0.52
319	41.0	0.318	–	–	–	–	–	–	–	–	–	–	0.74	0.77
320	–	–	–	–	–	–	–	–	–	–	–	–	1.00	1.16
322	–	–	–	–	–	–	–	–	–	–	–	–	0.69	0.70
323	–	–	–	–	–	–	–	–	–	–	–	–	0.5	0.52
324	44.3	0.420	–	–	–	–	–	–	–	–	–	–	1.08	1.18
325	42.5	0.364	–	–	–	–	–	(122)	–	–	–	–	–	–
326	40.7	0.309	64.2^q 64.7^{cc}	59.3	1674	1660	1058	100(99)	–	1733.4^u (1732.8)	1712.7	0.82	0.73	0.77
327	39.1	0.259	63.2^q	57.8	1673	1658	1055	106(108)	–	1731.7^u (1731.0)	1710.3	0.58	0.69	0.73
328	39.4	0.269	62.8^x	–	1672	1657	1055	108	–	–	–	0.92^n	–	–
329	37.7	0.216	–	–	1667	1656	1050	118	–	–	–	–	0.91	0.84
330	39.4	0.269	64.3^v	–	1671	1657	1053	–	–	–	–	0.95	0.88	0.89
331	36.4	0.176	–	–	–	–	–	–	–	–	–	0.62	0.57	0.61
332	–	–	–	–	–	–	–	–	–	–	–	–	0.72	0.76
333	(38.4)	(0.238)	–	–	–	–	–	–	–	–	–	–	0.40	0.47
334	37.2	0.201	–	–	–	–	–	–	–	–	–	–	–	–
335	–	–	–	–	–	–	–	–	–	–	–	–	0.68	0.74
336	(34.3)	(0.111)	–	–	–	–	–	–	–	–	–	–	–	–
337	–	–	–	–	–	–	–	–	–	–	–	–	0.24	–
338	kk	kk	–	–	–	–	–	–	–	–	–	–	–	–
339	32.8	0.065	–	–	1687	1664	1071	74(77)	1772.6	1741.2^u (1741.0)	1719.8	–	0.51	0.55
340	–	–	–	–	–	–	–	–	–	–	–	–	0.70	–
341	39.3	0.265	–	–	–	–	–	–	–	–	–	–	0.74	0.75
342	43.1	0.383	–	–	–	–	–	–	–	–	–	–	–	–
343	44.9	0.438	–	–	–	–	–	–	–	–	–	–	–	–
344	49.2 (40 °C)	0.571 (40 °C)	–	–	–	–	–	–	–	–	–	–	–	–
345	50.1	0.599	–	–	–	–	–	–	–	–	–	–	–	–
346	36.6	0.182	–	–	–	–	–	–	–	–	–	–	–	–

(a)Values taken from [1b] unless noted otherwise. All values at 25 °C, unless noted otherwise. Values in parentheses are secondary values as it is indicated in the text; (b) All values in kcal/mol; (c) Values, in kcal/mol; taken from [48]; (d) Values, in cm^{-1}; taken from [50]; (e) Values, in cm^{-1}; taken from [51]; (f) Values taken from [49]. Values in parentheses correspond to theG values measured in [52a]; (g) Values, in cm^{-1}, taken from [53]; (h) Values, in cm^{-1}, taken from [52b], unless noted otherwise; Values in parentheses are taken from [52d]; (i) Values, in cm^{-1}, taken from [52c]; (j) Values taken from [57], unless noted otherwise. Values in parentheses are estimated values; (k) Values taken from [17a]; (l) Calculated values from the wavenumber values of N,N-dimethyl-4-nitroaniline taken from [17a]; (m) Values taken from [60]; (n) Values taken from [55]; (o) Values taken from [56]; (p) Value based on methanol-ether and phenol-ether ROH···B solvent shifts; (q) Valtie taken from [33]; (r) Calculated value; (s) Value taken from [38]; (t) Value taken from [34]; (u) Values, in cm^{-1}; taken from [52c]; (v) Value taken from [39]; (w) Value taken from [40]; (x) Value taken from [36]; (y) Value taken from [1a]; (z) Value taken from [41]; (aa) Value taken from [31]; (bb) Value taken from [42]; (cc) Value taken from [35]; (dd) Value taken from [43]; (ee) Value taken from [44]; (ff) Calculated value, from [45]; (gg) In [48] this is the value corresponding to 4-methyl-2-pentanone, but it isa mistake, probably. (hh) Value taken from [46]; (ii) Calculated value, from [61] (jj) Value taken from [47]; (kk) Values taken from [31b] at different pressures are as follows:p (bar), $E_T(30)$, E_T^N; 150, 28.5, −0.068; 200, 29.0, −0.053; 250, 29.4, −0.040; 400, 32.2, 0.046; 500, 32.4, 0.053; 535, 32.5, 0.056; 550, 32.4, 0.053.

Table 2b

No.	σ(DMANF)[a]	σ(FNF)[a]	SPP[b]	SPP^{N} [b]	σ(**9**)[c]	σ(**10**)[c]	σ(**11**)[c]	σ(**12**)[c]	σ(**13**)[c]	σ(**14**)[c]	π^*_{azo} [d]	σ($C_{10}H_8$)[e]	σ($C_{14}H_{10}$)[f]	σ(β-car)[g]	π^*_2 [h]	σ(β-car) revised[i]
gas	(28231)	(32923)	−1.26	0.000	–	–	–	–	–	–	–	–	–	–	–	–
1	26595	31740	−0.78	0.214	–	–	–	–	–	–	–	–	–	–	–	–
9	24774	30798	0.16	0.629	–	–	–	–	–	–	–	–	–	–	–	22165
10	25387	31094	−0.18	0.479	–	–	–	–	–	–	–	32198	–	–	0.872	22364[j]
11	25290	31056	−0.11	0.507	–	–	–	–	–	–	–	32198	–	–	0.872	22331[j]
12	25191	30984	−0.09	0.519	20730[k]	19460[k]	22160[k]	20890[k]	21760[k]	21550[k]	−0.09[k]	32168	–	–	0.973	22232
13	25125	30931	−0.07	0.526	–	–	–	–	–	–	–	32169	–	–	0.970	–
14	25047	30888	−0.03	0.542	–	–	–	–	–	–	–	–	–	–	–	–
15	25163	30984	−0.05	0.533	–	–	–	–	–	–	–	32179	–	–	0.936	–
16	24978	30840	−0.01	0.552	–	–	–	–	–	–	–	–	–	22070	0.999	–
17	24925	30807	0.01	0.562	–	–	–	–	–	–	–	–	–	–	–	–
18	24934	30817	0.01	0.563	–	–	–	–	–	–	–	32139	–	–	1.071	–
19	24863	30764	0.03	0.571	–	–	–	–	–	–	–	–	–	21988	1.037	–
20	24792	30708	0.05	0.578	–	–	–	–	–	–	–	–	–	–	–	–
21	24814	30731	0.05	0.578	–	–	–	–	–	–	–	–	–	21905	1.076	–
22	24975	30802	−0.05	0.535	–	–	–	–	–	–	–	32160	–	–	1.000	–
23	24891	30764	0.00	0.517	20490	19360	21890	20690	21620	21620	0.00	32160	–	–	1.000	22008[j]
24	24759	30684	0.05	0.582	–	–	–	–	–	–	–	–	–	–	–	–
25	24661	30604	0.07	0.590	–	–	–	–	–	–	–	–	–	–	–	–
26	24931	30817	0.01	0.563	–	–	–	–	–	–	–	32154	–	–	1.020	22030[j]
30	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
31	–	–	–	–	–	–	–	–	–	–	–	32092[l]	–	–	1.230	–
33	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21603
35	24598	30564	0.10	0.601	–	–	–	–	–	–	–	–	–	21788	1.131	–
36	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21628
39	23913	30019	0.25	0.667	19730	18700	21240	20150	21150	20890	0.40	–	–	21575	1.230	–
40	23947	30028	0.22	0.655	19780	18710	21280	20150	21190	20920	0.38	–	–	–	–	21598
41	23930	29980	0.19	0.641	–	–	–	–	–	–	–	–	–	–	–	–
42	24123	30120	0.13	0.616	–	–	–	–	–	–	–	–	–	–	–	–
43	24141	30140	0.13	0.617	–	–	–	–	–	–	–	–	–	–	–	21673
44	24185	30097	0.04	0.576	–	–	–	–	–	–	–	–	–	–	–	–
46	24067	30136	0.21	0.650	–	–	–	–	–	–	–	–	–	–	–	–
48	–	–	–	–	–	–	–	–	–	–	–	–	–	21488	1.270	–

50	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21160
51	23836	29944	0.25	0.668	–	–	–	–	–	–	–	–	–	21434	1.296	–
52	24513	30544	0.17	0.632	–	–	–	–	–	–	–	–	–	21630	1.204	–
55	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21930
56	23258	29836	0.75	0.890	19080	18120	20800	19790	20970	20710	0.63	32123	–	–	1.125	21580
57	–	–	–	–	–	–	–	–	–	–	–	32118	–	–	1.142	21744
60	25067	31064	0.13	0.616	–	–	–	–	–	–	–	–	–	–	–	–
62	–	–	–	–	–	–	–	–	–	–	–	32108	–	–	1.176	–
63	–	–	–	–	–	–	–	–	–	–	–	32115	–	–	1.152	–
64	–	–	–	–	–	–	–	–	–	–	–	32073	–	–	1.294	–
65	–	–	–	–	–	–	–	–	–	–	–	32044	–	–	1.392	–
66	–	–	–	–	–	–	–	–	–	–	–	32164	–	–	0.986	–
67	–	–	–	–	–	–	–	–	–	–	–	32127	–	–	1.111	–
71	–	–	–	–	–	–	–	–	–	–	–	32102	–	–	1.196	–
73	23984	30449	0.63	0.837	–	–	–	–	–	–	–	32140	–	–	1.068	–
82	–	–	–	–	–	–	–	–	–	–	–	32031[f]	–	–	1.436	–
84	–	–	–	–	–	–	–	–	–	–	–	32120[f]	–	–	1.135	–
86	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	20475
87	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21413
89	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
91	23681	30003	0.48	0.769	–	–	–	–	–	–	–	–	–	–	–	21697
96	23764	30271	0.68	0.857	–	–	–	–	–	–	–	–	–	–	–	–
98	23288	29726	0.60	0.824	19280	18330	20920	19870	20940	20710	0.58	–	–	–	–	21409
99	22889	29511	0.80	0.911	–	–	–	–	–	–	–	–	–	–	–	–
106	23145	29584	0.60	0.824	–	–	–	–	–	–	–	–	26272	–	1.407	–
110	–	–	–	–	–	–	–	–	–	–	–	–	–	20999	1.498	–
112	23502	30091	0.76	0.895	18780	17990	20900	19930	20840	20850	0.63	32190[l]	–	–	0.899	22070
113	23525	30071	0.72	0.875	–	–	–	–	–	–	–	–	–	–	–	–
119	22842	29432	0.76	0.896	–	–	–	–	–	–	–	–	–	–	–	–
124	22693	29417	0.91	0.960	18670	17810	20530	19530	20490	20580	0.82	–	26278	–	1.399	–
129	24589	30751	0.31	0.694	19970	18770	21780	20480	21700	21310	0.16	32220[l]	–	–	0.797	22207
131	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	22183
132	24659	30733	0.21	0.652	–	–	–	–	–	–	–	–	–	–	–	–
135	23117	29544	0.59	0.819	–	–	–	–	–	–	–	–	–	–	–	–
136	24504	30669	0.31	0.695	–	–	–	–	–	–	–	–	–	–	–	–
137	24577	30724	0.29	0.687	–	–	–	–	–	–	–	–	–	–	–	–
141	23339	29775	0.60	0.823	–	–	–	–	–	–	–	–	–	–	–	–
147	–	–	–	–	19290	18220	21280	20050	21150	21100	0.45	–	–	–	–	–
148	23547	30051	0.67	0.855	–	–	–	–	–	–	–	–	–	–	–	–

COMMISSION ON PHYSICAL ORGANIC CHEMISTRY

Table 2b *Continued*

No.	σ(DMANF)[a]	σ(FNF)[a]	SPP[b]	SPP$^{\text{N}}$ [b]	σ(**9**)[c]	σ(**10**)[c]	σ(**11**)[c]	σ(**12**)[c]	σ(**13**)[c]	σ(**14**)[c]	π^*_{azo}[d]	$\sigma(C_{10}H_8)$[e]	$\sigma(C_{14}H_{10})$[f]	σ(β-car)[g]	π^*_2[h]	σ(β-car) revised[i]
151	23089	29591	0.67	0.854	–	–	–	–	–	–	–	–	–	–	–	–
155	23712	30181	0.63	0.838	–	–	–	–	–	–	–	–	–	–	–	21844
156	23563	29774	0.36	0.717	–	–	–	–	–	–	–	–	–	–	–	–
159	23945	30286	0.50	0.778	–	–	–	–	–	–	–	–	–	–	–	–
161	24118	30296	0.33	0.701	19750	18670	21220	20260	21430	21010	0.34	32144[f]	–	–	1.054	21725
167	23580	30139	0.73	0.881	19260	18090	21040	19970	20930	21050	0.53	–	26579	–	1.010	22046
168	23548	30106	0.73	0.881	18630	18140	21060	19920	20870	20870	0.61	–	–	–	–	21983
171	–	–	–	–	–	–	–	–	–	–	–	–	26568	–	1.024	–
172	23575	30139	0.73	0.883	–	–	–	–	–	–	–	–	26548	–	1.050	–
181	23279	29824	0.72	0.874	–	–	–	–	–	–	–	–	–	–	–	–
184	22776	(29445)	0.85	0.932	–	–	–	–	–	–	–	–	26272	–	1.407	–
189	23927	30323	0.56	0.804	–	–	–	–	–	–	–	–	–	–	–	–
190	24044	30400	0.52	0.785	19530	18460	21390	20180	20710	21060	0.44	–	–	–	–	–
202	23145	29608	0.63	0.836	–	–	–	–	–	–	–	–	–	–	–	–
206	24047	30423	0.54	0.795	19520	18450	21400	20230	21290	21040	0.37	–	–	22046	1.010	–
209	23241	29702	0.63	0.835	–	–	–	–	–	–	–	–	–	–	–	–
212	23946	30366	0.58	0.815	–	–	–	–	–	–	–	–	–	–	–	–
213	24047	30396	0.51	0.782	–	–	–	–	–	–	–	–	–	–	–	–
214	24067	30420	0.51	0.784	–	–	–	–	–	–	–	–	–	–	–	–
215	24172	30458	0.44	0.752	–	–	–	–	–	–	–	–	–	–	–	–
222	23059	29721	0.84	0.930	–	–	–	–	–	–	–	–	–	–	–	21734
223	22912	29695	0.97	0.987	–	–	–	–	–	–	–	–	–	–	–	–
225	23384	30025	0.82	0.920	–	–	–	–	–	–	–	–	–	–	–	–
231	22939	29652	0.90	0.954	18460	17430	20590	19580	20530	20480	0.86	–	–	21622	1.208	–
232	22902	29651	0.93	0.970	18420	17410	20660	19500	20560	20520	0.86	–	–	–	–	21642
234	23068	29749	0.86	0.939	–	–	–	–	–	–	–	–	–	–	–	–
235	23089	29752	0.84	0.930	–	–	–	–	–	–	–	–	–	–	–	–
238	23004	29715	0.89	0.952	–	–	–	–	–	–	–	–	–	–	–	–
241	–	–	–	–	18270	17270	20440	19260	20370	20270	(0.99)	–	–	–	–	–
242	22711	29458	0.93	0.970	–	–	–	–	–	–	–	–	–	–	–	–
250	23301	29876	0.75	0.889	–	–	–	–	–	–	–	–	–	–	–	–
251	23369	29985	0.79	0.908	–	–	–	–	–	–	–	–	–	–	–	–
255	22815	29481	0.85	0.932	18410	17400	20640	19430	20370	20850	(0.85)	–	–	–	–	21592

261	22557	29368	1.00	1.000	18230	17240	20340	19310	20240	20370	1.00	–	–	–	–	21372
263	22721	29538	1.00	1.003	–	–	–	–	–	–	–	–	–	–	–	–
267	22883	29528	0.82	0.922	18840	17840	20610	19530	20390	20590	0.80	–	–	21346	1.337	–
283	24824	30823	0.13	0.617	–	–	–	–	–	–	–	–	–	–	–	22041
284	24760	30775	0.15	0.624	–	–	–	–	–	–	–	–	–	–	–	–
287	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21263
288	24576	30586	0.15	0.622	–	–	–	–	–	–	–	–	–	–	–	–
289	22601	29307	0.89	0.950	–	–	–	–	–	–	–	–	–	–	–	–
292	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
296	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
303	23218	29833	0.79	0.907	18690	17880	20760	19870	20710	20750	(0.70)	–	26483	–	1.134	21844
304	23320	29907	0.76	0.894	–	–	–	–	–	–	–	–	26501	–	1.111	–
308	22463	(29290)	1.02	1.009	18500	17710	20390	19380	20330	20410	0.91	–	–	–	–	–
313	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	22168
320	22604	29073	0.63	0.838	–	–	–	–	–	–	–	–	–	–	–	–
321	23165	29743	0.75	0.890	–	–	–	–	–	–	–	–	–	–	–	–
324	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21039
325	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	21155
326	23263	29812	0.72	0.876	19140	18270	20870	19860	20710	20750	(0.62)	32114	–	–	1.155	21650
327	23405	29763	0.52	0.786	19290	18460	20780	19940	20710	20580	(0.62)	32090	–	–	1.236	21576[j]
329	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
330	22815	29386	0.74	0.887	–	–	–	–	–	–	–	32080	–	–	1.270	–
339	–	–	–	–	–	–	–	–	–	–	–	–	–	20730	1.624	–
346	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–

(a) Values, in cm^{-1}, taken from [59]; Values in parentheses are calculated values; (b) Values taken from [59]; (c) Values, in cm^{-1}, taken from [61]; (d) Values taken from [61]. Values in parentheses correspond to secondary values; (e) Values, in cm^{-1}, taken from [63] and collected in [62] unless noted otherwise; (D Values, in cm^{-1}, taken from [64a] and collected in [62]; (g) Values, in cm^{-1}, taken from [64b] and collected in [62]; (h) Values taken from [62]; (i) Values, in cm^{-1}, taken from [66] unless noted otherwise; (j) Value, in cm^{-1}, taken from [64b]; (k) Value corresponding toa mixture of hexane isomers; (l) Value, in cm^{-1}, taken from [65] and collected in [62].

Table 2c

No.	$\sigma_{OD}(K)$[a]	$\sigma_{OD}(S)$[b]	$B(KP)$[c]	$B(KP\text{-}S)$[d]	$B'(K\text{-}P)$[e]	$B'(PS)$[f]	β[g]	$\sigma(\mathbf{15})$[h]	$\sigma(\mathbf{16})$[h]	β_{OH}[i]	β_{NH2}[i]	$\sigma(NI)$[j]	$\sigma(MNI)$[j]	SB[k]	σ_{CO}[l]
gas	–	2720	0	0	0	–	–	–	–	–	–	31659[m]	30089[m]	0.000	1801.9
1	–	–	–	–	–	–	0.00	–	–	–	–	29921	28451	0.057	1796.6
2	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
3	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
7	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
8	–	–	–	–	–	–	–	–	–	–	–	–	–	–	1796.2
9	–	–	–	–	–	–	–	–	–	–	–	27273	25910	0.119	–
10	–	–	–	–	0	–	–	–	–	–	–	28950	27472	0.053	–
11	–	–	–	–	0	–	–	–	–	–	–	28919	27476	0.073	1790.8
12	2667	2696	–	24	0	–	0.00	–	–	–	–	28804	27331	0.056	–
13	2668	–	–	–	0	–	0.00	–	–	–	–	28672	27246	0.083	1790.1
14	–	–	–	–	0	–	–	–	–	–	–	28603	27171	0.079	–
15	–	–	–	–	0	–	–	–	–	–	–	28742	27249	0.044	–
16	–	–	–	–	0	–	–	–	–	–	–	28570	27092	0.053	–
17	–	–	–	–	0	–	–	–	–	–	–	28544	27088	0.066	–
18	–	–	–	–	0	–	–	–	–	–	–	–	–	–	–
19	–	–	–	–	0	–	–	–	–	–	–	28439	27018	0.086	–
20	–	–	–	–	0	–	–	–	–	–	–	28447	26996	0.068	–
21	–	–	–	–	0	–	–	–	–	–	–	28398	26978	0.086	–
22	–	–	–	–	0	–	–	–	–	–	–	28595	27134	0.063	–
23	–	2695	–	25	0	–	0.00	–	–	–	–	28545	27102	0.073	1789.1
24	–	–	–	–	0	–	–	–	–	–	–	28431	26980	0.069	–
25	–	–	–	–	0	–	–	–	–	–	–	28378	26942	0.077	–
26	–	–	–	–	0	–	–	–	–	–	–	28537	27103	0.078	–
28	–	–	–	–	97	–	–	–	–	–	–	–	–	–	–
35	–	–	–	–	0	–	–	–	–	–	–	28295	26823	0.056	–
36	–	–	–	–	0	–	–	–	–	–	–	–	–	–	–
37	–	–	–	–	0	–	–	–	–	–	–	–	–	–	–
39	2668	2668	52	52	48	–	0.10	33470	29090	0.10	0.03	26604	25249	0.124	1781.3
40	2666	2666	54	54	58	60	0.11	3590	9190	0.10	0.12	26733	25385	0.128	–
41	–	2661	–	59	68	–	–	–	–	–	–	26697	25399	0.157	–
42	–	2661	–	59	68	–	–	–	–	–	–	26818	25530	0.162	–
43	–	2662	–	58	68	–	–	3640	320	0.13	0.18	26855	25563	0.160	1781.0
44	–	2658	62	62	77	–	–	3550	9340	0.18	0.21	26878	25637	0.190	–

45	–	–	–	–	–	–	–	3460	9110	0.23	0.24	–	–	–	1779.5
46	2664	–	56	–	58	–	–	–	–	–	–	26798	25491	0.152	–
47	–	–	–	–	56	–	–	–	–	–	–	–	–	–	–
50	–	–	–	–	64^n	–	–	–	–	–	–	25520	24221	0.156	–
51	–	–	–	–	0	–	–	–	–	–	–	26587	25329	0.180	–
52	2689	2689	31	31	0	0	0.00	–	–	–	–	27978	26484	0.044	1786.4
56	2666	2671	54	49	40	–	0.00	–	–	–	–	25685	24334	0.126	–
57	–	–	–	–	–	–	0.00	–	–	–	–	26792	25370	0.085	–
60	–	–	–	–	–	–	–	–	–	–	–	28377	26873	0.038	–
63	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
64	–	–	–	–	10^n	–	0.00	–	–	–	–	–	–	–	–
65	–	–	–	–	2^n	–	0.00	–	–	–	–	–	–	–	1786.3
73	–	–	–	–	59	–	0.00	33810	29380	0.13	0.11	26783	25453	0.138	–
78	–	–	–	–	67	–	–	–	–	–	–	–	–	–	–
81	–	–	–	–	79^n	–	–	–	–	–	–	–	–	–	–
82	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
84	–	–	–	–	68	–	–	33670	29130	0.11	0.11	–	–	–	–
86	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
87	–	–	–	–	–	–	–	–	–	–	–	26028	24948	0.282	–
89	–	–	–	–	85	–	–	–	–	–	–	–	–	–	–
90	–	–	–	–	74	–	–	–	29040	–	0.07	–	–	–	–
91	–	2686	–	34	34	38	–	–	–	–	–	26387	25014	0.113	–
94	–	–	–	–	–	–	–	–	–	–	–	26741	25296	0.072	–
96	–	–	–	–	–	–	–	–	–	–	–	26518	25076	0.073	–
98	2670	2675	50	45	38	39	0.07	–	–	–	–	26060	24806	0.182	–
99	2679	2677	41	43	28	–	–	–	–	–	–	25705	24384	0.144	1782.0
100	2683	2678	37	42	17	–	–	–	–	–	–	–	–	–	–
105	–	–	–	–	37	–	–	–	–	–	–	–	–	–	–
106	2669	2671	51	49	40	–	0.06	–	–	–	–	25847	24609	0.191	–
107	–	–	–	–	–	–	–	–	–	–	–	–	–	–	1780.1
110	–	2667	49	53	38	–	–	–	–	–	–	25641	24345	0.158	–
112	2619	2617	101	103	160	157	0.31	32600	27500	0.39	0.37	25274	24200	0.286	1769.6
113	2616	–	104	–	162	–	0.37	–	–	–	–	25387	24451	0.365	–
114	–	–	–	–	164	–	–	–	–	–	–	25410	24503	0.384	–
115	–	–	–	–	–	–	–	–	–	–	–	25462	24595	0.408	–
119	–	–	–	–	–	–	–	32340	27280	0.18	0.17	24704	23453	0.184	1769.1
121	–	–	–	–	166	–	–	–	–	–	–	–	–	–	–
123	2631	–	–	–	139	–	–	–	–	–	–	–	–	–	–

Table 2c *Continued*

No.	$\sigma_{OD}(K)$[a]	$\sigma_{OD}(S)$[b]	B(KP)[c]	B(KP-S)[d]	B'(K-P)[e]	B'(PS)[f]	β[g]	$\sigma(\mathbf{15})$[h]	$\sigma(\mathbf{16})$[h]	β_{OH}[i]	β_{NH2}[i]	σ(NI)[j]	σ(MNI)[j]	SB[k]	σ_{CO}[l]
124	2630	2623	90	97	155	150	0.41	32090	27290	0.37	0.37	25036	23953	0.281	–
125	–	–	–	–	155	–	–	–	–	–	–	–	–	–	–
126	–	–	–	–	–	–	–	32050	27010	0.55	0.50	–	–	–	1761.0
129	2590	–	129	–	280	–	0.47	33220	28700	0.60	0.53	26774	26180	0.562	1762.8
130	2595	–	125	–	279	–	0.46	–	–	–	–	26837	26422	0.666	–
131	2593	2586	127	134	293	292	0.49	–	–	–	–	26885	26455	0.657	–
132	–	2591	129	129	285	267	0.46	33270	29040	0.66	0.49	26991	26527	0.637	1763.1
133	–	–	–	–	321	–	–	–	–	–	–	–	–	–	–
134	–	2663	–	57	123	–	0.13	–	–	–	–	–	–	–	–
135	–	–	–	–	233	–	0.41	32110	27760	0.46	0.30	25409	24412	0.330	–
136	–	–	–	–	263	–	–	–	–	–	–	26688	25995	0.505	–
137	–	–	–	–	295	–	–	–	–	–	–	26691	26104	0.567	–
138	–	–	–	–	298	–	–	–	–	–	–	–	–	–	–
140	2637	–	–	–	–	–	–	–	–	–	–	–	–	–	–
141	2642	2630–2659	78	75°	155	135	0.22	32860	28350	0.21	0.13	25658	24607	0.299	–
142	2643	2628–2660	77	76°	158	–	0.20	–	–	–	–	25865	24807	0.295	–
143	–	2565	155	155	–	331	–	–	–	–	–	25985	25693	0.737	–
144	–	–	–	–	178	–	–	32490	27670	0.31	0.28	–	–	–	–
145	–	–	–	–	223	–	–	–	–	–	–	–	–	–	–
147	2597	–	123	–	238	–	0.41	–	–	–	–	25554	25087	0.636	–
148	–	–	–	–	–	–	–	–	–	–	–	25365	24876	0.623	–
151	–	–	–	–	–	–	–	–	–	–	–	25143	24163	0.340	–
154	2664	–	56	–	103	–	–	–	–	–	–	26735	25351	0.107	–
155	2578	2575	142	145	287	285	0.55	32480	27710	0.59	0.48	25693	25148	0.591	–
156	–	–	–	–	–	–	–	–	–	–	–	25912	25356	0.584	–
157	–	–	–	–	–	–	–	–	–	–	–	26091	25606	0.625	–
158	–	–	–	–	–	–	–	32940	28250	0.71	0.67	–	–	–	–
159	2575	–	–	–	290	–	0.54	–	–	–	–	25887	25343	0.591	–
160	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
161	2591	2592	129	128	237	–	0.37	32880	28340	0.46	0.33	26074	25275	0.444	1760.8
162	2610	–	–	–	196	–	–	32670	27810	0.39	0.36	–	–	–	–
165	2609	–	–	–	–	–	–	–	–	–	–	–	–	–	–

166	2623	–	97	–	–	–	–	–	–	–	–	–	–	–	–
167	2604 2596[p]	2597	116	123	224	–	0.48	32500	27350	0.49	0.51	25359	24613	0.475	–
168	2611	2611	109	109	209	–	0.48	32420	27360	0.55	0.52	25440	24773	0.520	–
169	–	2618	–	102	–	–	0.48	–	–	–	–	–	–	–	–
170	–	2623	–	97	–	–	0.48	–	–	–	–	–	–	–	–
171	–	2609	–	111	–	–	0.50	–	–	–	–	–	–	–	–
172	2612 2619[p]	2620	108	100	–	–	0.45	–	–	–	–	25456	24853	0.557	–
173	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
174	–	2628	–	92	–	–	–	–	–	–	–	–	–	–	–
175	–	–	–	–	195	–	0.48	–	–	–	–	–	–	–	–
176	–	2609	–	111	210	–	–	–	–	–	–	–	–	–	–
180	–	2596	–	124	–	–	0.52	–	–	–	–	25211	24448	0..465	–
181	2602 2587[p]	2588	118	13	242	–	0.53	32140	27130	0.53	0.55	25206	24473	0.482	–
182	–	–	–	–	–	–	0.52	–	–	–	–	–	–	–	–
183	–	–	–	–	–	–	0.53	–	–	–	–	–	–	–	–
184	2612	2612	108	108	202	–	0.49	–	27090	–	0.45	249151	23978	0.365	–
186	–	–	–	–	–	–	0.14	–	–	–	–	–	–	–	–
189	–	–	–	–	–	–	0.37	–	–	–	–	25684	24846	0.422	–
190	2632	2632	88	88	170	–	0.42	32860	28020	0.52	0.41	25860	25205	0.527	–
191	2635	–	–	–	–	–	–	–	–	–	–	–	–	–	–
194	–	–	–	–	–	–	–	–	–	–	–	26252	25511	0.478	–
200	2638	–	–	–	163	–	–	–	–	–	–	–	–	–	–
201	2631	–	–	–	–	–	–	–	–	–	–	–	–	–	–
202	–	–	–	–	160	–	0.39	–	–	–	–	25368	24454	0.378	–
203	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
204	–	–	–	–	87[n]	–	–	–	–	–	–	–	–	–	–
205	–	–	–	–	–	–	0.36	–	–	–	–	–	–	–	–
206	2629	2631	91	89	181	–	0.45	32900	28100	0.50	0.43	25939	25309	0.542	–
209	–	–	–	–	142	–	0.41	–	–	–	–	25515	24669	0.417	–
210	–	–	–	–	125	–	0.35	–	–	–	–	–	–	–	–
211	–	–	–	–	–	–	0.25	–	–	–	–	–	–	–	–
212	–	–	–	–	–	–	–	–	–	–	–	25794	25176	0.549	–
213	–	–	–	–	–	–	–	–	–	–	–	25993	25374	0.548	–
214	–	–	–	–	158[n]	–	–	–	–	–	–	26083	25424	0.525	–
215	–	–	–	–	194	–	–	–	–	–	–	26244	25508	0.481	–

Table 2c *Continued*

No.	$\sigma_{OD}(K)$[a]	$\sigma_{OD}(S)$[b]	$B(KP)$[c]	$B(KP\text{-}S)$[d]	$B'(K\text{-}P)$[e]	$B'(PS)$[f]	β[g]	$\sigma(\mathbf{15})$[h]	$\sigma(\mathbf{16})$[h]	β_{OH}[i]	β_{NH2}[i]	$\sigma(NI)$[j]	$\sigma(MNI)$[j]	SB[k]	σ_{CO}[l]
216	2647	–	–	–	143	–	–	–	–	–	–	–	–	–	–
217	–	–	–	–	136	–	0.38	–	–	–	–	26070	25252	0.433	–
218	–	2635	85	85	145	154	0.40	33110	28580	0.45	0.38	26457	25477	0.340	–
219	–	–	–	–	190	–	–	–	–	–	–	–	–	–	–
222	–	–	–	–	–	–	0.40	–	–	–	–	24760	23781	0.341	–
223	2602	–	–	–	–	–	0.49	–	–	–	–	24705	23827	0.399	–
227	–	–	–	–	–	–	–	–	–	–	–	25576	24728	0.416	–
230	–	–	–	–	190	–	–	–	–	–	–	–	–	–	–
231	2561	2554	159	166	291	284	0.69	31430	26270	0.73	0.70	24434	23927	0.613	–
232	2555	2542	165	178	343	336	0.76	31330	26060	0.79	0.80	24421	23978	0.650	–
233	–	–	–	–	325	–	–	–	–	–	–	–	–	–	–
234	–	–	–	–	–	–	–	–	–	–	–	24662	24157	0.614	–
235	–	–	–	–	335	–	0.78	–	–	–	–	24715	24291	0.660	–
238	–	–	–	–	–	–	0.80	31500	26140	0.78	0.84	24117	24229	0.624	–
239	–	–	–	–	–	–	0.71	–	–	–	–	–	–	–	–
242	–	–	–	–	357[n]	–	0.77	31210	25950	0.76	0.78	24334	23828	0.613	–
250	–	–	–	–	–	–	–	31890	26600	0.66	0.66	24776	24111	0.522	1752.5
251	–	–	–	–	331	–	0.77	31840	26540	0.73	0.75	24958	24453	0.614	–
253	–	–	–	–	336[n]	–	–	–	–	–	–	–	–	–	–
254	–	–	–	–	–	–	–	32240	27080	0.57	0.57	–	–	–	1764.0
255	–	–	234	–	471	–	1.05	30850	25520	1.00	1.00	24234	24074	0.813	–
258	–	–	–	–	75	–	–	32860	27750	0.21	0.26	–	–	–	–
260	–	–	–	–	–	–	0.45	32570	27510	0.45	0.46	–	–	–	1770.2
261	2527	2528	193	192	362	358	0.76	31060	25750	0.73	0.73	23988	23541	0.647	–
262	–	–	–	–	–	–	0.80	30930	25680	0.76	0.75	–	–	–	–
263	–	–	–	–	157	–	–	32120 (30°C)	26850 (30°C)	0.33	0.37	24541	23604	0.365	–
266	–	–	–	–	152[n]	–	–	–	–	–	–	–	–	–	–
267	2500	2442–2478	220	260[o]	472	–	0.64	31090	26490	0.89	0.66	24583	24021	0.581	–
268	2485	2435–2466	235	270[o]	508	–	–	–	–	–	–	24906	24428	0.629	–
269	2508	2440–2470	–	265[o]	495	–	0.67	31100	26510	0.96	0.70	–	–	–	–

270	–	–	–	–	535	–	0.76	–	–	–	–	25248	24907	0.708	–
271	–	–	–	–	–	–	–	31070	26430	0.96	0.74	–	–	–	–
272	–	–	–	–	531	–	0.78	31410	26950	0.99	0.71	–	–	–	–
275	–	–	–	–	–	–	–	31890	27140	0.58	0.45	–	–	–	1753.9
276	–	–	–	–	–	–	–	32320	27640	0.41	0.31	–	–	–	1768.6
277	–	–	–	–	–	–	–	33620	29310	0.15	0.03	–	–	–	1776.9
279	–	–	–	–	–	–	–	31340	26770	0.62	0.45	–	–	–	–
280	–	–	–	–	–	–	0.51	31330	26880	0.73	0.55	–	–	–	–
281	–	–	–	–	–	–	0.48	–	26770	–	0.51	–	–	–	–
282	–	–	267^m	–	494	–	0.64	–	26350	–	0.57	24251	23594	0.526	–
283	2430	2406	290	314	650	–	0.71	32500	28830	1.16	0.65	26805	26771	0.885	–
284	–	–	–	–	–	–	0.62	32460	29460	1.21	0.49	26952	26864	0.854	–
285	–	–	–	–	–	–	0.71	32140	28160	1.16	0.76	26212	26374	0.998	–
286	–	–	–	–	–	–	0.57	31850	28210	1.01	0.55	–	–	–	–
287	2520	–	200	–	422	–	–	–	–	–	–	25392	24352	0.305	–
288	–	–	–	–	727	–	–	–	–	–	–	26508	26389	0.836	–
289	–	–	–	–	–	–	0.82	–	–	–	–	23887	23458	0.658	–
290	–	–	–	–	–	–	–	32250	28210	1.01	0.67	25863	25736	0.832	–
291	–	–	–	–	–	–	–	33100	28560	0.33	0.21	–	–	–	1766.8
292	–	–	–	–	251	–	–	33190	28740	0.37	0.31	–	–	–	1767.4
293	–	–	–	–	–	–	–	33330	28980	0.43	0.34	–	–	–	1768.6
294	–	–	–	–	252	–	–	33310	29020	0.44	0.34	–	–	–	1767.5
295	–	–	–	–	–	–	–	–	–	–	–	–	–	–	1768.6
296	–	–	–	–	–	–	–	–	28350	–	0.13	–	–	–	1772.7
297	–	–	–	–	–	–	–	–	28640	–	0.13	–	–	–	1773.9
298	–	–	–	–	–	–	–	32690	28060	0.33	0.25	–	–	–	–
300	–	–	–	–	–	–	–	32790	28110	0.37	0.28	25692	24878	0.436	1764.1
301	–	–	–	–	–	–	–	32910	28410	0.38	0.22	–	–	–	–
302	–	–	–	–	–	–	–	–	28150	–	0.13	25497	24268	0.197	1768.7
303	2662	2661	58	59	65	–	–	–	–	–	–	25068	23907	0.236	–
304	2660	–	60	–	66	–	–	–	–	–	–	25340	24176	0.234	–
305	–	–	–	–	68	–	–	–	–	–	–	–	–	–	–
306	–	–	–	–	73	–	–	–	–	–	–	–	–	–	–
308	2647	2657	73	63	67	65	0.39	–	–	–	–	24954	23801	0.240	–
309	–	–	–	–	537	–	0.72	–	–	–	–	25329	25397	0.944	–
312	–	–	–	–	–	–	0.57	–	–	–	–	–	–	–	–
313	–	–	–	–	637	–	–	–	–	–	–	–	–	–	–
314	–	–	–	–	597	–	–	–	–	–	–	–	–	–	–

Table 2c *Continued*

No.	$\sigma_{OD}(K)$[a]	$\sigma_{OD}(S)$[b]	$B(KP)$[c]	$B(KP\text{-}S)$[d]	$B'(K\text{-}P)$[e]	$B'(PS)$[f]	β[g]	$\sigma(\mathbf{15})$[h]	$\sigma(\mathbf{16})$[h]	β_{OH}[i]	β_{NH2}[i]	$\sigma(NI)$[j]	$\sigma(MNI)$[j]	SB[k]	σ_{CO}[l]
316	–	–	–	–	–	–	–	–	–	–	–	25190	25284	0.959	–
317	–	–	–	–	–	–	–	–	–	–	–	25555	25590	0.925	–
318	2428	2421–	292	290[o]	706	–	–	–	–	–	–	25377	25425	0.933	–
	–	2438	–	–	–	–	–	–	–	–	–	–	–	–	–
319	–	–	–	–	–	–	–	–	–	–	–	24901	24390	0.610	–
320	–	–	–	–	343	–	–	–	–	–	–	24143	22883	0.179	–
321	–	–	–	–	114	–	–	–	–	–	–	25374	24227	0.244	–
324	2510	2511	210	209	346	–	–	–	–	–	–	23919	22808	0.264	–
325	2517	2536	203	184	452	–	–	–	–	–	–	24580	23378	0.212	–
326	2680	2677	40	43	23	–	0.00	–	–	–	–	25559	24298	0.178	–
327	2685	2681	35	39	14	–	0.00	–	–	–	–	25938	24492	0.071	–
	–	–	–	–	–	–	0.00	–	–	–	–	–	–	–	–
329	–	–	–	–	32[n]	–	–	–	–	–	–	–	–	–	–
330	–	–	–	–	29[n]	–	0.00	–	–	–	–	25347	23806	0.017	–
331	–	–	–	–	12[n]	–	0.00	–	–	–	–	–	–	–	–
334	–	–	–	–	80	–	–	–	–	–	–	–	–	–	–
339	–	–	–	–	–	–	–	–	–	–	–	26629	25239	0.104	1738.8
341	–	–	–	–	–	–	–	–	25750	–	1.04	24381	24546	1.000	–

(a) Values, in cm^{-1}, taken from [69]; (b) Values, in cm^{-1}, taken from [70]; (c) Values, in cm^{-1}, taken from [13]; (d) Values, in cm^{-1}, taken from [70]; (e) Values, in cm^{-1}, taken from [71], unless noted otherwise; (f) Values, in cm^{-1}, taken from [73]; (g) Values taken from [57]; (h) Values, in cm^{-1}, taken from [75]; (i) Calculated values. See text; (j) Values, in cm^{-1}, taken from [78]; (k) Values taken from [78]; (l) Values, in cm^{-1}, taken from [53]; (m) Calculated value; (n) Value, in cm^{-1}, taken from [72]; (o) Mean value obtained from the two bands; (p) Value measured by T. Kagiya and reported in [70].

Table 2d

No.	$\Delta\sigma_{CO}$[a]	σ_{HgBr}[b]	D_S[c]	μ_M[d]	SP[e]	DN[f]	$-\Delta H°_{BF_3}$[g]	A[h]	B[h]	S'[i]
gas	–	221.8	–	–	–	–	–	–	–	–
12	–	–	–	–	–	0.0	–	0.01 ± 0.02	−0.01 ± 0.02	–
13	–	–	–	–	–	0.0	–	0.00 ± 0.00	0.00 ± 0.00	–
15	–	–	–	–	–	–	–	0.01 ± 0.02	−0.03 ± 0.08	–
23	–	–	–	–	–	0.0	–	0.02 ± 0.02	0.06 ± 0.01	1.11
39	1.4	213	9	–	–	0.1	–	0.15 ± 0.01	0.59 ± 0.02	1.73
40	–	–	–	–	–	0.1	–	0.13 ± 0.01	0.54 ± 0.02	1.66
41	–	–	–	–	–	–	–	0.06 ± 0.04	0.53 ± 0.02	–
42	–	–	–	–	–	5.0	–	0.04 ± 0.05	0.50 ± 0.02	–
43	3.4	–	–	–	–	5.0	–	0.06 ± 0.03	0.50 ± 0.02	–
44	–	–	–	–	–	10.0	–	–	–	–
45	5.1	–	–	–	–	–	–	–	–	–
52	–	–	–	–	–	0.0	–	0.09 ± 0.02	0.34 ± 0.02	1.49
55	–	–	–	0.07	–	–	–	–	–	–
56	–	215	7	0.03	–	0.1	–	0.30 ± 0.02	0.82 ± 0.02	–
57	–	–	–	–	–	–	–	–	–	(1.93)
64	–	–	–	–	–	–	–	0.16 ± 0.05	0.54 ± 0.03	(1.90)
65	–	–	–	–	–	–	–	0.10 ± 0.03	0.25 ± 0.03	–
91	–	–	–	–	–	3.0	–	–	–	–
98	–	–	–	–	–	3.3	–	0.20 ± 0.02	0.65 ± 0.02	2.07
99	–	–	–	–	–	3.0	–	–	–	(2.13)
100	–	–	–	–	–	2.0	–	–	–	–
106	–	–	–	–	–	3.0	–	0.22 ± 0.02	0.66 ± 0.02	–
110	–	–	–	–	–	4.0	–	–	–	–
112	11.7	209.5	12	0.34[j]	32	14.6 ± 0.1[k,l] 14.1	60.39 ± 0.46	0.37 ± 0.01	0.86 ± 0.02	3.00
113	–	207.5	14	0.36[m]	33	16.1[l]	60.95 ± 0.21	–	–	(2.80)
114	–	209	13	0.37[m]	30	16.6[l]	61.18 ± 0.28	–	–	–
119	8.4	–	–	–	–	10.0	44 ± 2[n]	–	–	–
121	–	–	–	–	–	–	60.92 ± 0.13	–	–	–
124	–	210	12	0.36[j]	25	13.0 ± 0.2[k,l] 11.9	55.44 ± 0.28	0.30 ± 0.02	0.87 ± 0.03	2.63
125	–	–	–	0.38[j]	–	15.1[l]	56.61 ± 0.23	–	–	–
126	19.4	–	–	–	–	17.0	77.23 ± 0.61[n]	–	–	(2.81)
129	23.8	210	12	–	–	19.2[l]	78.77 ± 0.38	0.12 ± 0.02	0.34 ± 0.02	1.73
130	–	–	–	–	–	17.84 ± 0.02[o] 18.0	79.42 ± 0.27	–	–	–
131	–	–	–	–	–	19.0	76.61 ± 0.39	–	–	–
132	24.1	–	–	–	–	19.0	78.57 ± 0.39	0.06 ± 0.02	0.28 ± 0.03	1.58
135	–	–	–	–	–	19.0	–	–	–	–
141	–	212	10	–	–	9.0	–	0.21 ± 0.02	0.74 ± 0.03	(2.04)[p]
142	–	–	–	–	–	8.0	–	–	–	–
143	–	–	–	–	–	24.0	–	–	–	–
144	–	–	–	–	–	16.0	–	–	–	–
147	–	–	–	–	–	20.0	–	0.21 ± 0.02	0.50 ± 0.11	–
154	–	212	10	–	–	6.0	–	–	–	–
155	–	204.5	17	0.00[m]	–	20.5 ± 0.5[l,q] 21.03 ± 0.05[o] 20.0	90.40 ± 0.28	0.17 ± 0.01	0.67 ± 0.02	2.08
156	–	–	–	–	–	12.0	–	–	–	–
159	–	–	–	–	–	22.0	85.36 ± 0.46	–	–	1.98
161	20.8	204	18	–	–	14.8	74.09 ± 0.27	0.19 ± 0.01	0.67 ± 0.02	1.93
162	–	–	–	–	–	–	68.63 ± 0.43[n]	–	–	–
167	–	207	15	0.03	–	17.03 ± 0.04[l,o] 17.0	76.03 ± 0.21	0.25 ± 0.01	0.81 ± 0.03	2.58
168	–	–	–	–	–	17.43 ± 0.03[l,o] 17.4	76.07 ± 0.33	0.23 ± 0.02	0.74 ± 0.03	2.51
169	–	–	–	–	–	17.07 ± 0.03[l,o]	74.84 ± 0.25	–	–	–
170	–	–	–	–	–	16.95 ± 0.03[l,o]	72.83 ± 0.37	–	–	–

Table 2d *Continued*

No.	$\Delta\sigma_{CO}$[a]	σ_{HgBr}[b]	D_S[c]	μ_M[d]	SP[e]	DN[f]	$-\Delta H°_{BF3}$[g]	A[h]	B[h]	S'[i]
171	–	–	–	–	–	17.50 ± 0.02[l,o]	76.19 ± 0.37	–	–	–
172	–	–	–	–	–	16.53 ± 0.03[l,o]	72.28 ± 0.23	–	–	–
						15.0				
174	–	–	–	–	–	16.20 ± 0.03[l,o]	68.07 ± 0.74	–	–	–
175	–	–	–	–	–	9.64 ± 0.07	31.32 ± 0.41	–	–	–
177	–	–	–	–	–	–	73.28 ± 0.49	–	–	–
179	–	–	–	–	–	–	70.70 ± 0.57	–	–	–
180	–	–	–	–	–	18.0	77.44 ± 0.45	–	–	–
181	–	–	–	–	–	17.79 ± 0.01[l,o]	76.36 ± 0.82	0.25 ± 0.03	0.79 ± 0.04	2.35
	–	–	–	–	–	18.0	–	–	–	–
184	–	–	–	–	–	15.0	74.52 ± 0.15	0.23 ± 0.02	0.90 ± 0.03	2.52
189	–	–	–	–	–	–	69.76 ± 0.11	–	–	–
190	–	210	12	–	–	16.38 ± 0.04[l,o]	72.79 ± 0.33	–	–	(2.35)
						16.5				
191	–	–	–	–	–	11.0	–	–	–	–
202	–	–	–	–	–	15.0	59.4 ± 1.1	–	–	–
205	–	–	–	–	–	17.00 ± 0.07[l,o]	71.17 ± 0.29	–	–	–
206	–	–	–	–	–	17.08 ± 0.04[l,o]	75.55 ± 0.31	0.21 ± 0.02	0.59 ± 0.02	2.15
						16.6 ± 0.3[k]				
						17.1				
209	–	–	–	–	–	15.0	61.2 ± 0.8	–	–	–
210	–	–	–	–	–	13.0	–	–	–	–
213	–	–	–	–	–	16.0	–	–	–	–
214	–	–	–	–	–	15.0	–	–	–	–
217	–	–	–	–	–	15.17 ± 0.03[l,o]	67.63 ± 0.38	–	–	–
						17.2				
218	–	–	–	–	–	15.98 ± 0.05[l,o]	71.03 ± 0.35	–	–	–
						16.0				
220	–	–	–	–	–	16.4	–	–	–	–
222	–	212	12	−0.09	–	14.91 ± 0.07[l,o]	64.19 ± 0.39	–	–	(3.10)[r]
						15.1				
223	–	208	14	0.02[j]	–	18.0	–	–	–	(2.86)[p]
225	–	–	–	–	–	10.5	–	–	–	–
231	–	198	24	0.11	–	26.6	110.49 ± 0.18	0.30 ± 0.01	0.93 ± 0.03	2.80
232	–	198	24	0.17	–	27.8 ± 0.03[l,o]	112.14 ± 0.41	0.27 ± 0.02	0.97 ± 0.04	2.70
						27.8				
234	–	–	–	0.09	–	30.9[l]	113.20 ± 0.35	–	–	–
235	–	198	24	0.17	–	32.2[l]	113.61 ± 0.25	–	–	–
236	–	170	52	1.33[j]	107	–	–	–	–	–
238	–	198	24	0.14	–	29.64 ± 0.03[l,o]	108.62 ± 0.22	–	–	(2.48)
						29.6				
240	–	–	–	–	–	–	114.16 ± 0.57	–	–	–
241	–	–	–	–	–	–	112.13 ± 0.29	–	–	–
242	–	195	27	0.13	–	27.3[l]	112.56 ± 0.36	–	–	2.62
						28.2[s]				
243	–	166	56	1.36[j]	115	–	–	–	–	–
246	–	–	–	–	–	27.1	–	–	–	–
250	27.2	199	23	0.02[m]	–	23.0[l]	84.75 ± 0.22	–	–	(2.79)
251	–	–	–	–	–	26,.0	–	–	–	(2.55)[p]
253	–	199.5	22	–	–	23.7	–	0.00 ± 0.00	1.07 ± 0.05	(2.30)
254	17.8	–	–	–	–	–	–	–	–	–
255	–	188	34	0.29	–	38.8	117.53 ± 0.45	–	–	2.52
						50.3[s]				
256	–	169	53	0.67	89	–	–	–	–	–
259	–	–	–	–	–	–	51.27 ± 0.46	–	–	–
260	12.4	–	–	–	–	–	55.13 ± 0.77	–	–	–
261	–	194	28	0.22	–	29.8[l]	105.34 ± 0.36	0.34 ± 0.02	1.08 ± 0.04	3.60
262	–	193	29	–	–	–	–	–	–	–
263	–	207	15	0.00	–	14.8[l]	51.32 ± 0.29	–	–	(2.88)[r]

Table 2d *Continued*

No.	$\Delta\sigma_{CO}$[a]	σ_{HgBr}[b]	D_S[c]	μ_M[d]	SP[e]	DN[f]	$-\Delta H°_{BF3}$[g]	A[h]	B[h]	S'[i]
267	–	184	38	0.66[j]	–	34.0 ± 0.4[k,l] 34.1 ± 0.4[t,u] 33.1	128.08 ± 0.50	0.24 ± 0.02	0.96 ± 0.04	2.44
268	–	183	39	–	–	–	123.44 ± 0.47	–	–	–
269	–	183	39	–	–	34.0	134.17 ± 0.59	–	–	–
270	–	–	–	–	–	–	97.73 ± 0.58	0.18 ± 0.02	0.81 ± 0.08	–
272	–	–	–	–	–	–	101.03 ± 0.29	–	–	–
274	–	–	–	–	–	–	96.20 ± 0.29[n]	–	–	–
275	27.1	–	–	–	–	–	–	–	–	–
276	13.6	–	–	–	–	–	–	–	–	–
277	4.7	–	–	–	–	–	–	–	–	–
282	–	–	–	–	–	32.0	–	–	–	(2.30)[r]
283	–	–	23[v]	–	–	31.7 ± 0.6[l,t,u] 48.4[s] 60.9[x]	135.87 ± 1.67	0.08 ± 0.03	0.19 ± 0.04	(1.43)[p]
284	–	–	–	–	–	50.0	–	–	–	–
286	–	–	–	–	–	21.0	–	–	–	–
287	–	–	–	–	–	27.0	109.16 ± 0.76	–	–	(1.96)
291	16.3	–	–	–	–	–	–	–	–	–
292	17.0	–	–	–	–	–	–	–	–	–
293	17.1	–	–	–	–	–	–	–	–	–
294	17.7	181	41	–	–	–	–	–	–	–
295	17.8	–	–	–	–	–	–	–	–	–
296	8.6	–	–	–	–	–	–	–	–	–
297	9.3	–	–	–	–	–	–	–	–	–
299	–	–	–	–	–	–	–	–	–	(1.83)
300	17.7	179	43	0.80	73	–	51.62 ± 0.20[n]	–	–	(1.99)
302	11.5	–	–	–	–	–	–	–	–	–
303	–	213	9	0.03	–	2.7	37.63 ± 0.56	0.39 ± 0.02	0.92 ± 0.03	3.07
304	–	–	–	–	–	–	–	–	–	(2.78)
308	–	213	9	0.23	–	8.1 ± 0.7[l,o] 4.4	35.79 ± 1.40	0.29 ± 0.02	0.86 ± 0.03	2.61
309	–	–	–	–	–	42.0	–	0.15 ± 0.04	1.17 ± 0.06	–
310	–	–	–	–	–	57.5	–	–	–	–
313	–	–	–	–	–	50.0	–	–	–	–
318	–	174	48	–	–	40.0	–	–	–	–
320	–	–	–	0.81[m]	–	–	–	–	–	–
324	–	188	34	~0.75[m]	–	35.0	–	0.36 ± 0.02	1.19 ± 0.05	–
325	–	–	–	–	–	33.0	–	0.40 ± 0.03	1.07 ± 0.05	–
326	–	216	6	–	–	1.0	10.0 ± 3.0	0.33 ± 0.01	0.80 ± 0.03	–
327	–	–	–	–	–	4.0	–	0.42 ± 0.01	0.73 ± 0.02	–
339	–	–	–	–	–	2.0	–	0.10 ± 0.02	0.38 ± 0.02	(1.51)[p]
340	–	–	–	–	–	11.7	–	–	–	–

(a) Values, in cm^{-1}, taken from [53]; (b) Values, in cm^{-1}, taken from [79]; (c) Values taken from [79]; (d) Values taken from [80], unless noted otherwise; (e) Values taken from [82]; (f) Values, in kcal/mol, taken from [83] and collected in [36], unless noted otherwise; (g) Values, in kJ/mol, taken from [84]; (h) Values taken from [93]; (i) Values taken from [94]; (j) Value taken from a personal ommunication from Prof. Y. Marcus; (k) Value, in kcal/mol, taken from [86] and collected in [84]; (l) Value recommended in [84]; (m) Value taken from [81]; (n) Value, in kJ/mol, taken from [92]; (o) Value, in kcal/mol, taken from [87] and collected in [84]; (p) Limited data available; (q) Value, in kcal/mol, taken from [88] and collected in [84]; (r) Calculated from betaine shift only; (s) Value, in kcal/mol, taken from [90] and collected in [84]; (t) Value, in kcal/mol, taken from [89] and collected in [84]; (u) Value measured in CH_2Cl_2 solution, at 218 K; (v) Estimated from ν_S(Hg-I); (x) Value, in kcal/mol, taken from [91] and collected in [84].

GENERAL COMMENTS ON THE SCALES

In general terms and as a first approximation, the electrostatic, nonspecific part of solvation can be described in terms of the orientation and polarization components of the reaction field. Dispersive interactions are also of fundamental importance. For practical purposes, the spirit of some of the criteria set forth by Koppel & Palm [13] and Palm & Palm [14] seem appropriate at this point. Thus, we consider the orientation component of the solvent polarization to be appropriately described by the function $[g(\varepsilon_r) - f(n)]$ while the atomic and electronic polarization part, together with dispersive interactions, can be described by $f(n)$. Thus, for solvents such as those examined here, we can expect 'overall solvation' scales as well as 'polarity-polarizability' scales to be amenable to a treatment as linear combinations of these two functions. Thus, for the value taken in a given medium by any such scale, SC, eqn 42 is expected to hold:

$$SC = af(n) + b[g(\varepsilon_r) - f(n)] + c \tag{42}$$

wherein a, b and c are constants. We present in Table 3 the results of such a treatment. It is clear that the various scales presented here generally follow eqn 42 to a significant degree of precision. In the worst cases, removal of just a few data points leads to quite respectable correlation coefficients. Notice that the range of ratios b/a is quite broad. This, of course, is one of the reasons behind the proliferation of scales over the years.

It is reasonable to suggest that any study of medium effects on a given property be carried out first using $f(n)$ and $[g(\varepsilon_r) - f(n)]$ separately and then as linear combination of both and avoiding solvents in which substantial 'specific' interactions (hydrogen bonding and/or donor-acceptor effects) can be expected to be important on account of the nature of the solute and/or the property under scrutiny. Then, after consideration of the b/a ratio, the use of various empirical scales can be explored. Notice that in the case of the π^* scale, some specific interactions involving polychlorinated and aromatic solvents are likely to be present. They are dealt with in the $\underline{d}\delta$ formalism characteristic of this method [3].

As regards the scales of hydrogen bonding and Lewis basicities, we have selected β_{OH} as an appropriate reference in order to explore the mutual correlations of the other scales. As indicated earlier, two factors are needed in order to describe 'basicity'. Thus, in view of the relatively poor correlation between β_{OH} and D_s or μ_M, a preliminary exploration using these scales seems in order. This should allow to narrow the field of the search. It should be kept in mind that, very often, correlations of 'basicity' effects with any of the various single parameter basicity scales reported herein leads to a clear display of family dependence. This should not be overlooked, as it is physically important. Of course, care should be exercised when comparing very small data sets because chemically unsound results can be obtained.

(Regarding the correlations portrayed in Table 3b and 3c. Prof. Gritzner [79b] has expressed his concern about these correlations on account of the paucity of soft-soft systems in the general database. We feel that, in any case, these correlations are useful as they show the present statistical status of the matter. Of course, the reader should not use them without proper consideration of the physical meaning of the various scales. More extensive discussions of these problems, including discussion of data for hydroxylic solvents are given in [95].)

We conclude by reminding the reader that this compilation provides more scales and properties than generally used for the purpose of the treatment of 'medium effects'. One of the main reasons for this is the concept that scales and physical magnitudes should be selected considering their physical meaning and the *similarity principle* [15]. Appropriate choices would lead to a deeper understanding of the role of the solvent [96].

Table 3a Results of the correlations between different scales and the functions $f(n)$ and $[g(\varepsilon_r) - f(n)]$. Correlations are in form: $y = a x + b$ and $z = a x + b y + c$

Scales	$f(n)$	$[g(\varepsilon_r) - f(n)]$	$f(n), [g(\varepsilon_r) - f(n)]$
$E_T(30)$	a = 6.3 ± 5.8 b = 35.8 ± 2.1 $n = 190$ $r = 0.079$ u = 4.1	a = 17.34 ± 0.72 b = 32.19 ± 0.29 $n = 190$ $r = 0.869$ u = 2.0	a = 13.1 ± 2.7 b = 17.65 ± 0.69 c = 27.5 ± 1.0 $n = 190$ $r = 0.884$ u = 1.9
		a = 16.59 ± 0.59 b = 32.24 ± 0.23 $n = 182$ $r = 0.903$ u = 1.6 (excluding gas and solvents # 185, 186, 207, 216, 220, 324 and 325)	a = 12.6 ± 2.1 b = 17.02 ± 0.54 c = 27.61 ± 0.81 $n = 181$ $r = 0.921$ u = 1.5 (excluding solvents # 123, 185, 186, 207, 216, 220, 272, 324 and 325)
Z	a = −44 ± 16 b = 79.1 ± 5.7 $n = 46$ $r = 0.375$ u = 3.9	a = 14.5 ± 2.7 b = 57.7 ± 1.2 $n = 45$ $r = 0.637$ u = 3.2	a = −27 ± 14 b = 13.2 ± 2.7 c = 67.7 ± 5.2 $n = 45$ $r = 0.676$ u = 3.1
		a = 15.1 ± 2.4 b = 57.3 ± 1.1 $n = 41$ $r = 0.711$ u = 2.7 (excluding solvents # 156, 161, 189 and 222)	a = −38 ± 11 b = 12.4 ± 2.2 c = 71.5 ± 4.0 $n = 39$ $r = 0.797$ u = 2.3 (excluding solvents # 156, 161, 169, 222, 261 and 263)
Z'	a = 29 ± 31 b = 71 ± 10 $n = 16$ $r = 0.247$ u = 4.1	a = 12.1 ± 4.8 b = 55.4 ± 2.3 $n = 16$ $r = 0.562$ u = 3.5	a = −8 ± 29 b = 11.6 ± 5.2 c = 58 ± 11 $n = 16$ $r = 0.566$ u = 3.6
G	a = 221 ± 37 b = 1 ± 13 $n = 35$ $r = 0.720$ u = 17.0	a = 67 ± 17 b = 62.5 ± 5.4 $n = 35$ $r = 0.564$ u = 20.3	a = 209 ± 25 b = 60.4 ± 9.8 c = −10.0 ± 9.4 $n = 35$ $r = 0.883$ u = 11.7
	a = 221 ± 30 b = −2 ± 11 $n = 29$ $r = 0.822$ u = 13.1 (excluding solvents # 12, 23, 112, 303, 325 and 327)	a = 49 ± 11 b = 66.6 ± 3.6 $n = 30$ $r = 0.642$ u = 12.6 (excluding gas and solvents # 3, 325, 327 and 329)	a = 189 ± 17 b = 63.4 ± 6.3 c = −6.7 ± 6.1 $n = 31$ $r = 0.948$ u = 7.4 (excluding solvents # 161, 325, 327 and 329)
π^*	a = 4.30 ± 0.42 b = −0.92 ± 0.15 $n = 97$ $r = 0.724$ u = 0.25	a = 1.14 ± 0.14 b = 0.191 ± 0.057 $n = 92$ $r = 0.649$ u = 0.28	a = 4.22 ± 0.17 b = 1.103 ± 0.051 c = −1.268 ± 0.063 $n = 92$ $r = 0.962$ u = 0.10
	a = 3.55 ± 0.37 b = −0.62 ± 0.13 $n = 87$ $r = 0.725$ u = 0.20 (excluding solvents # 1, 2, 3, 8, 12, 13, 23, 65, 112 and 303)	a = 0.868 ± 0.096 b = 0.322 ± 0040 $n = 83$ $r = 0.707$ u = 0.18 (excluding gas and solvents # 1, 2, 3, 8, 86, 135, 203 and 287)	a = 4.14 ± 0.15 b = 1.113 ± 0.044 c = −1.240 ± 0.056 $n = 86$ $r = 0.971$ u = 0.084 (excluding solvents # 3, 8, 39, 73, 110 and 161)
	a = 2.49 ± 0.46 b = −0.23 ± 0.17 $n = 86$ $r = 0.510$ u = 0.19 (excluding gas and solvents # 1, 2, 3, 8, 12, 13, 23, 65, 112 and 303)		
SPP^N	a = 1.81 ± 0.31 b = 0.13 ± 0.11 $n = 95$ $r = 0.518$ u = 0.15	a = 0.646 ± 0.039 b = 0.558 ± 0.015 $n = 91$ $r = 0.870$ u = 0.089	a = 1.604 ± 0.070 b = 0.625 ± 0.015 c = 0.016 ± 0.024 $n = 91$ $r = 0.983$ u = 0.034
		a = 0.598 ± 0.022 b = 0.580 ± 0.009 $n = 87$ $r = 0.945$ u = 0.050 (excluding gas and solvents # 1, 135 and 151)	a = 1.521 ± 0.057 b = 0.625 ± 0.015 c = 0.016 ± 0.024 $n = 89$ $r = 0.988$ u = 0.027 (excluding solvents # 1 and 161)
π^*_{azo}	a = 3.6 ± 1.4 b = −0.67 ± 0.48 $n = 25$ $r = 0.476$ u = 0.26	a = 0.99 ± 0.17 b = 0.173 ± 0.081 $n = 25$ $r = 0.765$ u = 0.19	a = 4.38 ± 0.48 b = 1.083 ± 0.082 c = −1.38 ± 0.17 $n = 25$ $r = 0.956$ u = 0.088
		a = 0.81 ± 0.16 b = 0.264 ± 0.073 $n = 20$ $r = 0.769$ u = 0.15 (excluding solvents # 12, 129,	a = 4.47 ± 0.43 b = 1.149 ± 0.078 c = −1.44 ± 0.16 $n = 24$ $r = 0.965$ u = 0.080

		167, 241 and 261)	(excluding solvents # 161)
π^*_2	a = 3.85 ± 0.23 b = −0.213 ± 0.082	a = 0.04 ± 0.11 b = 1.131 ± 0.038 n = 48 r = 0.053 u = 0.18	a = 4.00 ± 0.21 b = 0.143 ± 0.037 c = −0.300 ± 0.075
	n = 49 r = 0.925 u = 0.068 a = 4.15 ± 0.22 b = −0.315 ± 0.079 n = 45 r = 0.942 u = 0.055 (excluding solvents # 65, 110, 129 and 303)		n = 48 r = 0.945 u = 0.059 a = 4.04 ± 0.19 b = 0.168 ± 0.027 c = −0.320 ± 0.068 n = 44 r = 0.959 u = 0.042 (excluding solvents # 65, 110, 129 and 339)
$\sigma(\beta\text{-car})$	a = −7675 ± 447 b = 24446 ± 160 n = 37 r = 0.945 u = 133	a = −228 ± 298 b = 21799 ± 108 n = 37 r = 0.13 u = 404	a = −7940 ± 291 b = −452 ± 64 c = 24668 ± 108 n = 37 r = 0.957 u = 86
S'	a = 3.11 ± 0.68 b = −2.3 ± 1.9 n = 46 r = 0.18 u = 0.49	a = 2.20 ± 0.16 b = 1.382 ± 0.074 n = 46 r = 0.901 u = 0.22	a = 1.85 ± 0.86 b = 2.32 ± 0.16 c = −0.68 ± 0.33 n = 46 r = 0.914 u = 0.21

Table 3b Results of the correlations between different scales and the β_{OH} scale. Correlations are in the form: $y = a\ x + b$

Scales	β_{OH}
$B(KP)$	a = 212 ± 16 b = 13.1 ± 9.5; n = 22 r = 0.949 u = 19.6 a = 195 ± 16 b = 22.0 ± 8.9; n = 20 r = 0.947 u = 17.0 (excluding solvents # 190 and 283)
$B(KP–S)$	a = 239 ± 19 b = 7 ± 11 n = 22 r = 0.942 u = 24.8 a = 229 ± 16 b = 14.1 ± 9.5; n = 19 r = 0.959 u = 20.5 (excluding solvents # 190, 206 and 267)
$B'(K–P)$	a = 499 ± 23 b = −11 ± 14; n = 36 r = 0.964 u = 39.2 a = 493 ± 18 b = −8 ± 10; n = 30 r = 0.981 u = 27.4 (excluding solvents # 141, 190, 218, 231, 283 and 292)
$B'(PS)$	a = 404 ± 44 b = 16 ± 24; n = 10 r = 0.956 u = 31.1
β	a = 0.642 ± 0.076 b = 0.122 ± 0.054; n = 34 r = 0.832 u = 0.13 a = 1.052 ± 0.055 b = −0.059 ± 0.032; n = 26 r = 0.969 u = 0.063 (excluding solvents # 267, 269, 272, 280, 283, 284, 285 and 286)
β_{NH2}	a = 0.674 ± 0.051 b = 0.082 ± 0.031; n = 60 r = 0.868 u = 0.11 a = 0.747 ± 0.040 b = 0.046 ± 0.022; n = 53 r = 0.933 u = 0.075 (excluding solvents # 232, 238, 242, 255, 283, 284 and 286)
	a = 0.984 ± 0.043 b = −0.039 ± 0.022; n = 51 r = 0.957 u = 0.066 (excluding solvents # 267, 269, 271, 272, 283, 284, 285, 286 and 290)
SB	a = 0.715 ± 0.033 b = 0.087 ± 0.021; n = 35 r = 0.967 u = 0.060 a = 0.730 ± 0.031 b = −0.083 ± 0.019; n = 34 r = 0.973 u = 0.054 (excluding solvent # 267)
D_S	a = 20.5 ± 7.5 b = 10.4 ± 5.0; n023 r = 0.513 u = 9.3 a = 34.3 ± 3.9 b = 0.3 ± 2.5; n = 20 r = 0.902 u = 4.1 (excluding solvents # 283, 294 and 300)
μ_M	a = −0.03 ± 0.33 b = 0.26 ± 0.22; n = 14 r = 0.030 u = 0.25
$-\Delta H^\circ_{BF3}$	a = 104.9 ± 7.3 b = 21.2 ± 4.8; n = 29 r = 0.941 u = 8.9 a = 111.7 ± 6.5 b = 17.9 ± 4.1; n = 28 r = 0.959 u = 7.6 (excluding solvent # 272)
	a = 125.8 ± 5.7 b = 12.0 ± 3.4; n = 24 r = 0.978 u = 5.2 (excluding solvents # 132, 255, 260, 272 and 283)

Table 3c Results of correlations between different scales and the -$\Delta H°_{BF3}$ scale. Correlations are in the form: y = a x + b

Scales	$-\Delta H°_{BF3}$
D_S	a = 0.221 ± 0.044 b = 2.4 ± 4.0; *n* = 27 *r* = 0.708 u = 7.5
	a = 0.255 ± 0.027 b = −1.7 ± 2.5; *n* = 26 *r* = 0.887 u = 4.6
	(excluding solvent # 300)
	a = 0.262 ± 0.024 b = −2.2 ± 2.1; *n* = 24 *r* = 24 *r* = 0.916 u = 3.8
	(excluding solvents # 268, 283 and 300)
μ_M	a = −0.0004 ± 0.0016 b = 0.25 ± 0.14; *n* = 22 *r* = 0.055 u = 0.22
DN	a = 0.282 ± 0.012 b = −2.9 ± 1.0; *n* = 50 *r* = 0.959 u = 2.2
	a = 0.2644 ± 0.0094 b = −1.6 ± 0.78; *n* = 48 *r* = 0.972 u = 1.7
	(excluding solvents # 255 and 303)

Table 3d Results of correlations between A and B scales. Correlations are in the form: y = a x + b

Scales	*B*
A	a = 0.272 ± 0.039 b = 0.014 ± 0.028; *n* = 43 *r* = 0.734 u = 0.082
	a = 0.310 ± 0.021 b = −0.004 ± 0.015; *n* = 37 *r* = 0.927 u = 0.041
	(excluding solvents # 42, 112, 253, 303, 309 and 327)

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APPENDIX

Some symbols, acronyms and abbreviations used in this text

DMANF   2-(dimethylamino)-7-nitrofluorene

DMSO   dimethylsulfoxide

FNF   2-fluoro-7-nitrofluorene

HB   Hydrogen bond

HBA   Hydrogen bond acceptor

HBD   Hydrogen bond donor

HMPA   Hexamethylphosphorictriamide

KAT   Kamlet, Abboud, Taft

MNI   1-methyl-5-nitroindoline

n   number of data points (in correlations)

NI   5-nitroindoline

r   correlation coefficient

SCM   Solvatochromic comparison method

TMG   Tetramethylguanidine

TMS   Tetramethylsilane

u   Standard deviation