



Relation between the characteristic molecular volume and hydrophobicity of nonpolar molecules

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ABSTRACT

Experimental values of the Gibbs free energies of hydration for a set of nonpolar or very slightly polar compounds are analyzed in order to investigate how does the hydrophobic effect depend on molecular structure and shape. The contribution due to the hydrophobic effect is evaluated using a method we suggested previously. A number of values of the Gibbs free energies of solvation in dimethyl sulfoxide and in hexadecane, which are required for calculation, were determined by gas chromatographic headspace analysis. It is found that the Gibbs hydrophobic effect energy is linearly dependent on characteristic molecular volume for a large variety of solutes with branched and unbranched carbon chains, different functional groups and atomic composition. Molecular structure and shape do not significantly affect the hydrophobicity of chemical species, and molecular volume is a main factor determining it.

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1. Introduction

The hydrophobic effect is being intensively studied using both theoretical and experimental methods [1–3]. One of the important questions is how the structure of a molecule relates to its hydrophobicity.

Thermodynamic functions of hydration of solute A Δ_{hydr}^A ($f = G, H, S$) are greatly influenced by the hydrophobic effect. Their experimental values are a good starting point to analyze this phenomenon using various models of hydration. Alternatively, one can study hydration of idealized objects such as hard particles in computer simulations. The energy of hydration of a hard particle is the cavitation energy of water. Using Monte-Carlo methods [4] and information theory approaches [5], it was shown that the Gibbs free energy of hydration of relatively small hard spherical particles is proportional to the volume of a particle (for molarity-based standard states). The study of hydration of non-spherical hard particles with different shape [6] also showed that the Gibbs free energy of hydration is primarily governed only by the volume of a particle.

Real solutes behave very differently from hard particles. A plot of the Gibbs free energies of hydration *versus* molecular or molar volumes of real solutes cannot be approximated by a single curve [7]: different classes of nonpolar solutes (e.g. alkanes, arenes, and noble gases) lie on different straight lines with different slopes and intercepts. This is because real solutes engage in different degrees of intermolecular interactions with water. For solutes with-

out the ability of hydrogen-bonding or donor–acceptor bonding, these interactions are called nonspecific interactions. Their energy is dependent on solute structure.

The question of whether and how intermolecular interactions influence the hydrophobicity of real molecules has not been answered. It is necessary to analyze the values of Δ_{hydr}^A using some extrathermodynamic model in order to distinguish the effects caused by the hydrophobic effect from those caused by nonspecific interactions. In the present work, we report a thermodynamic analysis of experimental Gibbs free energies of hydration for a number of nonpolar compounds to investigate how does the hydrophobic effect depends on molecular structure and shape.

2. Methodology

Recently, we suggested [8] that a dramatic difference between magnitudes of the Gibbs free energy of hydration of nonpolar solutes and their Gibbs free energy of solvation in ‘regular’ solvents can be expressed in terms of the Gibbs energy of the hydrophobic effect, $\Delta_{\text{h.e.}}G^A$. The Gibbs free energy of hydration can be considered as the sum of the Gibbs energy of the hydrophobic effect and the Gibbs nonspecific hydration energy, $\Delta_{\text{hydr(nonsp)}}G^A$. Here and below the energies are at $T = 298 \text{ K}$; the molar fraction scale of concentration is used and the standard pressure is 1 bar. The last quantity can be calculated using a general empiric equation for the Gibbs nonspecific solvation energy, which has been shown [9] to be correct for various non-associated solvents. This equation is given by:

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$$\Delta_{\text{solv(nonsp)}}G^{A/S} = \Delta_{\text{solv}}G^{A/S_0} + (\delta g^S - \delta g^{S_0}) \cdot V_x^A + \left[a + b(\delta g^S)^{1/2} \right] \cdot \left[(\Delta_{\text{solv}}G^{A/S_R} - \Delta_{\text{solv}}G^{A/S_0}) - (\delta g^{S_R} - \delta g^{S_0}) \cdot V_x^A \right]; \quad (1)$$

$$a = -(\delta g^{S_0})^{1/2} / \left[(\delta g^{S_R})^{1/2} - (\delta g^{S_0})^{1/2} \right];$$

$$b = 1 / \left[(\delta g^{S_R})^{1/2} - (\delta g^{S_0})^{1/2} \right].$$

Here $\Delta_{\text{solv}}G^{A/S_0}$ and $\Delta_{\text{solv}}G^{A/S_R}$ are the Gibbs free energies of solvation of solute A in the standard solvents S_0 and S_R (typically hexadecane and dimethyl sulfoxide), δg^S , δg^{S_R} , and δg^{S_0} are solvent parameters reflecting nonspecific interactions of solvent molecules with other (solvent and solute) molecules, and V_x^A is McGowan's characteristic volume of solute A, which can be calculated by a simple additive scheme from atomic contributions [10]. (For example, the molecule of benzene has $V_x^{\text{C}_6\text{H}_6} = 6 \cdot 0.1635$ (volume of 6 carbons) + $6 \cdot 0.0871$ (volume of 6 hydrogens) – $12 \cdot 0.0656$ (negative contribution from 12 chemical bonds) = $0.7164 \text{ cm}^3 \cdot \text{mol}^{-1} \cdot 10^2$.) The values of parameter δg for water, dimethyl sulfoxide, and hexadecane are, respectively ($5.8 \cdot 10^{-2}$, $10.1 \cdot 10^{-2}$, and $0.0 \cdot 10^{-2}$) $\text{kJ} \cdot \text{cm}^{-3}$.

The values of $\Delta_{\text{h.e.}}G^A$ have been determined using the following equation:

$$\Delta_{\text{h.e.}}G^A = \Delta_{\text{hydr}}G^A - \Delta_{\text{hydr(nonsp)}}G^A \quad (2)$$

for solutes forming no energetically significant hydrogen bonds with water in aqueous solutions.

In equation (1), a single solvent parameter δg^S is used to describe both the nonspecific interactions of solvent molecules with each other and those between solvent and solute molecules. This equation gives an acceptable accuracy ($\sigma = 0.85 \text{ kJ} \cdot \text{mol}^{-1}$ for 676 systems [9]) when one tries to predict the Gibbs free energies of solvation for the systems where no solute-solvent hydrogen bonding or the hydrophobic effects take place. In aqueous systems, the strength of interactions between water molecules is greater than that between water and solute molecules, so a single parameter cannot be used to describe both kinds of interactions. Parameter $\delta g^{\text{H}_2\text{O}}$ reflects the ability of water for the nonspecific interactions with solutes, and the additional Gibbs free energy of the hydration process due to the strong interactions between molecules of water is reflected by the hydrophobic effect term $\Delta_{\text{h.e.}}G^A$.

For a set of 30 different molecules (including noble gases, alkanes, arenes, and their halogenated derivatives), the Gibbs hydrophobic effect energy has been found to be linearly dependent on the characteristic molecular volume V_x^A [8]:

$$\Delta_{\text{h.e.}}G^A / (\text{kJ} \cdot \text{mol}^{-1}) = 22.5V_x^A / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot 10^2) + 3.5 \quad (n = 30, \sigma = 1.02 \text{ kJ mol}^{-1}, r^2 = 0.9901). \quad (3)$$

In our present work, we extend this methodology to a number of nonpolar or very slightly polar compounds that contain different functional groups: double and triple bonds, rings, halogen atoms, and/or have a non-linear hydrocarbon chain. The task is to check whether the Gibbs energy of the hydrophobic effect is related only to volume effects and is independent of molecular structure and shape. While alkanes cannot form hydrogen bonds with proton donors, multiple bonds and halogen atoms may form such bonds with a molecule of water. However, these bonds are weak. Moreover, it is necessary to break or reorganize strong water-water bonds in order to form a solute-water bond in aqueous solution. Thus we believe that the contribution of hydrogen bonding with water is negligible for all species considered – only a small per cent of solute molecules will participate in such bonds.

To perform calculations by equations (1) and (2), one needs to know an experimental value of $\Delta_{\text{hydr}}G^A$ and the Gibbs free energies of solvation in DMSO and hexadecane. There is a huge amount of data on aqueous solubility and the Gibbs free energy of hydration of various species [11–14]. The Gibbs free energies of solvation in hexadecane were also measured for many different compounds [15], while the Gibbs free energies of solvation in DMSO are unknown in most cases. In the present work we experimentally determined the Gibbs free energies of solvation for a number of the molecules considered in DMSO and in a few cases also in hexadecane in order to calculate $\Delta_{\text{hydr(nonsp)}}G^A$ and then $\Delta_{\text{h.e.}}G^A$.

3. Experimental

The Gibbs free energies of solvation are related to measurable limiting activity coefficients of solute A in solvent S, $\gamma^{A/S}$, through the equation: $\Delta_{\text{solv}}G^{A/S} = RT \ln (\gamma^{A/S} p_{\text{sat}}^A)$, where p_{sat}^A is the saturated vapor pressure of pure A in bar. We measured $\gamma^{A/S}$ at 298 K using gas chromatographic head space analysis (Chromatex Crystall-2000M chromatograph, quartz glass column with an HP-5 stationary phase). Design of the automatic electropneumatic dosing system used for head space sampling has been described before [16]. The gas phase samples were taken from vials of 15 ml volume containing 1 ml of solution or pure compound. The values of $\gamma^{A/S}$ were calculated from the ratio of vapor pressure of solute A over its solution in S ($p_A^{A/S}$) and p_{sat}^A : $\gamma^{A/S} = p_A^{A/S} / (p_{\text{sat}}^A x_A^{A/S})$, where $x_A^{A/S}$ is the molar fraction of A in solution. The ratio $p_A^{A/S} / p_{\text{sat}}^A$ is equal to the ratio of areas of chromatographic peaks in two subsequent head space analyses of pure A and its solution. When calculating $\gamma^{A/S}$, a correction of initial concentration on the quantity of evaporated solute was made. The molar fractions of solutes in solutions lied in the interval 0.002 to 0.04. For solutes with rather low volatility, we also conducted experiments at one order lower concentrations. For all studied systems, measurements were made at three different concentrations of A, and repeated 2 times for each concentration. An average value of the Gibbs free energy rounded to $0.1 \text{ kJ} \cdot \text{mol}^{-1}$ was taken. In all systems studied there was no significant concentration dependence of $\gamma^{A/S}$ (the difference between any pair of experimental values did not exceed 10 per cent, or $0.3 \text{ kJ} \cdot \text{mol}^{-1}$ in the Gibbs free energy units). The maximum standard uncertainties for a single (solute + solvent) system are: $\sigma(\ln \gamma^{A/S}) = 0.05$, $\sigma(\Delta_{\text{solv}}G^{A/S}) = 0.12 \text{ kJ} \cdot \text{mol}^{-1}$. The average standard uncertainties are: $\sigma(\ln \gamma^{A/S}) = 0.03$, $\sigma(\Delta_{\text{solv}}G^{A/S}) = 0.07 \text{ kJ} \cdot \text{mol}^{-1}$. For example, measured activity coefficients of 4-isopropyltoluene in DMSO at different concentrations are given in table 1. Saturated vapor pressures of pure compounds needed for calculation were taken from EPI Suite program database [17].

All chemicals were pure grade (Aldrich and Fluka). DMSO was dried using 4 Å molecular sieves and distilled in vacuo. Hexadecane was purified by fractional crystallization.

Results of the measurements are given in table 2.

TABLE 1

Measured values of the activity coefficient at different concentrations and corresponding Gibbs free energies of solvation for 4-isopropyltoluene in DMSO at $T = 298 \text{ K}$

Experiment number	$x_A^{A/S}$	$\gamma^{A/S}$	$\Delta_{\text{solv}}G^{A/S}/(\text{kJ} \cdot \text{mol}^{-1})$
1	0.000457	15.53	–8.67
2	0.00455	15.35	–8.69
3	0.00455	14.64	–8.81
4	0.00905	15.04	–8.74
5	0.00905	15.17	–8.72
6	0.0135	14.75	–8.79
7	0.0135	15.41	–8.68

($\Delta_{\text{solv}}G^{A/S}) = -8.73 \text{ kJ} \cdot \text{mol}^{-1}$, $\sigma(\Delta_{\text{solv}}G^{A/S}) = 0.05 \text{ kJ} \cdot \text{mol}^{-1}$, $\sigma(\ln \gamma^{A/S}) = 0.02$.)

TABLE 2

Measured values of limiting activity coefficients at $T = 298$ K and corresponding Gibbs free energies of solvation.

Solute (A)	Solvent (S)	$\gamma_{\infty}^{A/S}$	$\Delta_{\text{sol}}G^{A/S}/(\text{kJ} \cdot \text{mol}^{-1})$
1,5-Hexadiene	DMSO	11.6	3.0
1,5-Hexadiene	Hexadecane	0.80	-3.6
1-Heptyne	DMSO	6.9	-1.8
1-Hexyne	DMSO	4.1	-0.8
1-Octyne	DMSO	10.2	-4.2
4-Isopropyltoluene	DMSO	15.1	-8.7
4-Vinyl-1-cyclohexene	DMSO	20.7	-2.1
4-Vinyl-1-cyclohexene	Hexadecane	0.96	-9.7
Bromotrichloromethane	DMSO	2.1	-5.5
Cycloheptatriene	DMSO	5.7	-4.3
Cyclohexene	DMSO	14.9	1.4
Cyclooctane	DMSO	63.3	-1.9
Cyclooctane	Hexadecane	0.96	-12.3
Cyclopentene	DMSO	7.0	3.1
Methylcyclohexane	DMSO	49.2	2.7
Methylcyclopentane	DMSO	29.5	4.2
Tetrachloroethene	DMSO	10.5	-3.3

4. Results and discussion

Results of calculation are presented in table 3. The Gibbs free energies of hydration were taken from the literature or calculated from the literature values of aqueous solubilities or limiting activity coefficients [12,13,18–20]. The Gibbs free energies of solvation in hexadecane in most cases were also calculated from the literature data on gas-hexadecane distributions [15]. The systematic errors in experimental energies of solvation in nonaqueous solvents, judging on the basis of comparison of results obtained by different authors, rarely exceed $1 \text{ kJ} \cdot \text{mol}^{-1}$. Solubility measurements in water sometimes have greater uncertainty; we have tried

to choose the most reliable data, e.g. those in agreement with the reference values from IUPAC-NIST solubility data series.

In figure 1, the Gibbs hydrophobic effect energies from table 3 are plotted against characteristic molecular volumes. A line corresponding to correlation (3) observed previously [8] for 30 different solutes is also shown. One can see that the data points do not significantly deviate from this line. The root mean square deviation from equation (3) is $1.16 \text{ kJ} \cdot \text{mol}^{-1}$, while the RMS of equation (3) itself was $1.02 \text{ kJ} \cdot \text{mol}^{-1}$.

Results of our previous work [8] (the values of $\Delta_{\text{h.e.}}G^A$ for 30 solutes, including noble and simple gases, linear alkanes, aromatic hydrocarbons and their halogenated derivatives, see table 4) and the newly calculated values from table 3 can be brought together, and a single correlation with V_x^A is obtained. It is given by:

$$\Delta_{\text{h.e.}}G^A/(\text{kJ} \cdot \text{mol}^{-1}) = (22.02 \pm 0.36)V_x^A/(\text{cm}^3 \cdot \text{mol}^{-1} \cdot 10^2) + (3.65 \pm 0.33) \quad (4)$$

$(n = 58, \sigma = 1.09 \text{ kJ} \cdot \text{mol}^{-1}, r^2 = 0.9847).$

The characteristic molecular volume V_x^A used in correlations is a simple and effective measure of molecular volumes. It can be calculated by an atom-additive scheme and correlates with van der Waals volumes of molecules.

The united set of molecules includes 58 species that belong to different classes of organic compounds as well inorganic substances. They contain different functional groups, have branched and unbranched carbon chains, rings, and different heteroatoms. However, neither structure nor shape significantly affects the values of $\Delta_{\text{h.e.}}G^A$, which is driven by molecular volume. Similarly, the Gibbs free energy of hydration of hard particles with different shape that do not interact with water was shown [6] to be linearly dependent on the volume of particles, which is in agreement with our results. We can now conclude that nonspecific interactions also do not alter the hydrophobicity of molecules.

This conclusion relates only to the Gibbs free energy and not to other thermodynamic functions. In contrast, the enthalpies of the hydrophobic effect that we determined previously [23], are structure-sensitive. It is evident that the enthalpic effects of structure on solute hydrophobicity should be compensating with the entropic ones. These effects may be a result of water reorganization processes.

TABLE 3

Calculated values of the Gibbs hydrophobic effect energies for a set of solutes and the data used for their calculation by equations (1) and (2)^a.

Solute (A)	$V_x^A \cdot 10^{-2}/(\text{cm}^3 \cdot \text{mol}^{-1})$	$\Delta_{\text{hydr}}G^A/(\text{kJ} \cdot \text{mol}^{-1})$	$\Delta_{\text{sol}}G^{A/\text{DMSO}}/(\text{kJ} \cdot \text{mol}^{-1})$	$\Delta_{\text{sol}}G^{A/\text{C}_{16}\text{H}_{34}}/(\text{kJ} \cdot \text{mol}^{-1})$	$\Delta_{\text{h.e.}}G^A/(\text{kJ} \cdot \text{mol}^{-1})$
1,2-Dichlorobenzene	0.9612	11.8 ^f	-12.3 ⁱ	-14.8 ^e	26.4
1,5-Hexadiene	0.8680	22.3 ^b	3.0 ^g	-3.6 ^a	22.4
1-Heptyne	1.0089	20.5 ^b	-1.8 ^g	-6.1 ^e	25.2
1-Hexene	0.9110	24.8 ^c	5.8 ^h	-3.7 ^e	23.0
1-Hexyne	0.8680	19.1 ^b	-0.8 ^g	-3.3 ^e	22.1
1-Octyne	1.1498	20.9 ^b	-4.2 ^g	-9.1 ^e	28.3
2,2,4-Trimethylpentane	1.2358	31.0 ^c	5.1 ^h	-6.7 ^e	31.1
2,3,4-Trimethylpentane	1.2358	28.8 ^c	3.6 ^h	-8.9 ^e	30.5
2,4-Dimethylpentane	1.0949	28.4 ^c	5.7 ^h	-5.0 ^e	27.3
2-Methylpentane	0.9540	28.4 ^c	7.0 ^h	-3.3 ^e	25.6
4-Isopropyltoluene	1.2800	17.0 ^c	-8.7 ^g	-15.2 ^e	29.6
4-Vinyl-1-cyclohexene	1.0412	19.4 ^c	-2.1 ^g	-9.7 ^e	25.2
Acenaphthene	1.2586	4.6 ^c	-23.1 ^h	-25.9 ^e	30.6
Bromotrichloromethane	0.7917	14.0 ^d	-5.5 ^g	-7.7 ^d	21.4
Carbon tetrachloride	0.7391	17.0 ^e	-0.9 ^h	-5.1 ^e	20.2
Cycloheptatriene	0.8573	14.0 ^c	-4.3 ^g	-8.6 ^e	20.9
Cyclohexene	0.8024	19.4 ^e	1.4 ^g	-6.2 ^e	21.4
Cyclooctane	1.1272	21.5 ^c	-1.9 ^g	-12.3 ^a	28.0
Cyclopentene	0.6615	19.5 ^c	3.1 ^g	-2.7 ^e	19.0
Ethylbenzene	0.9982	14.8 ^c	-5.6 ^h	-10.6 ^e	23.5
Isoprene	0.7271	21.2 ^c	4.6 ^h	-1.0 ^e	19.3
Methylcyclohexane	0.9863	24.7 ^c	2.7 ^g	-8.0 ^e	26.4
Methylcyclopentane	0.8454	24.3 ^c	4.2 ^g	-5.1 ^e	24.0
Methylene chloride	0.4943	12.4 ^e	-2.7 ^h	-0.5 ^e	15.4
Tetrachloroethene	0.8370	16.8 ^f	-3.3 ^g	-9.5 ^e	23.2
Toluene	0.8573	14.5 ^c	-4.4 ^h	-8.0 ^e	21.3
Phenanthrene	1.4544	0.7 ^c	-31.9 ^h	-32.5 ^e	35.3
Pyrene	1.5846	-1.8 ^c	-38.6 ^h	-39.4 ^e	39.7

^a All Gibbs free energies are at 298 K.

^b Calculated from limiting activity coefficients assembled in [18].

^c Calculated from reference values of aqueous solubility from IUPAC-NIST solubility data series [12].

^d From reference [20].

^e Calculated from gas-hexadecane distribution constants reported in [15].

^f Calculated from limiting activity coefficients in [13].

^g Calculated from limiting activity coefficients measured in [19].

^h Taken from compilation [21].

ⁱ Measured in [22].

^{*} Values obtained in the present work.

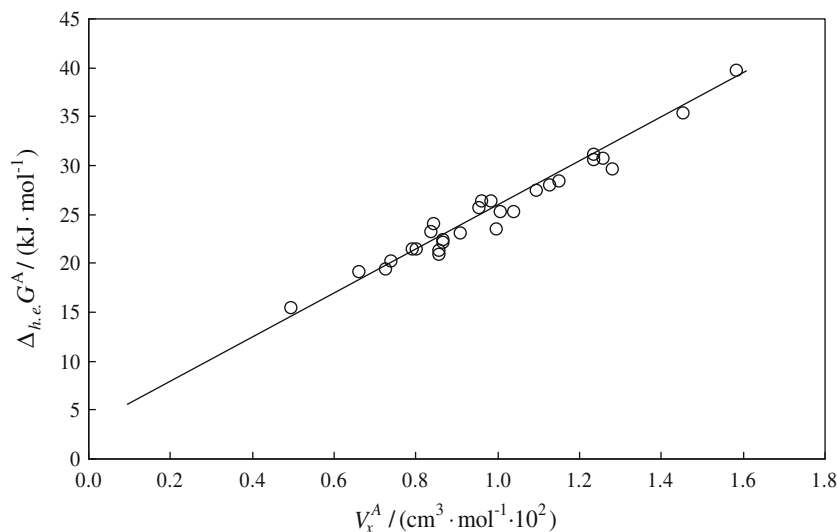


FIGURE 1. Gibbs energy of the hydrophobic effect at 298 K for compounds from table 3 versus characteristic molecular volume of a solute. A straight line corresponds to equation (3).

TABLE 4

Values of the Gibbs hydrophobic effect energies for different molecules calculated in reference [8].

Solute (A)	$V_x^A / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot 10^2)$	$\Delta_{h,e}G^A / (\text{kJ} \cdot \text{mol}^{-1})$	Solute (A)	$V_x^A / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot 10^2)$	$\Delta_{h,e}G^A / (\text{kJ} \cdot \text{mol}^{-1})$
He	0.0680	5.2	Heptane	1.0949	29.2
Ne	0.0850	5.6	Octane	1.2358	32.8
Ar	0.1900	7.0	Nonane	1.3767	35.9
Kr	0.2460	8.2	Decane	1.5176	38.1
Xe	0.3290	10.3	Cyclohexane	0.8454	22.9
H ₂	0.1086	6.2	(E)-1,2-Dichloroethene	0.5922	17.1
N ₂	0.2222	7.4	(Z)-1,2-Dichloroethene	0.5922	16.8
O ₂	0.1830	7.2	Benzene	0.7164	18.2
Methane	0.2495	9.3	Fluorobenzene	0.7341	19.4
Ethane	0.3904	13.4	Chlorobenzene	0.8388	22.1
Propane	0.5313	16.3	Bromobenzene	0.8914	23.0
Butane	0.6722	19.8	Iodobenzene	0.9746	25.3
Isobutane	0.6722	19.1	Naphthalene	1.0854	26.3
Pentane	0.8131	22.7	Biphenyl	1.3242	30.8
Hexane	0.9540	26.0	Anthracene	1.4540	34.6

Equations (2) and (3) may be applied to compounds that form hydrogen bonds with water. Equation (3) is correct for molecules containing different kinds of atoms, including such molecules as N₂ and O₂. Now, if we consider, for instance, organic substances containing nitrogen or oxygen atoms, it is reasonable to suppose that the Gibbs free energy of hydration of non-hydrogen bonded form of these substances will be described by the same equations (2) and (3). In such cases, by subtracting the calculated value for non-bonded form from the experimental Gibbs free energy of hydration, one can find the Gibbs free energy of hydrogen bonding with water [24], which is not possible to determine using direct methods.

Another possible use of equations (2) and (3) is prediction of the values of $\Delta_{\text{hydr}}G^A$ and related quantities such as aqueous solubility, Henry's law constants, and gas-water distribution coefficients for various non-hydrogen bonding substances. These are difficult to measure directly because of low solubility, however, these quantities are important for the studies of toxicity, biological activity and distribution of these compounds in natural systems.

5. Conclusion

Cyclic and acyclic hydrocarbons with double, triple and single C–C bonds, π -conjugated compounds and aromatic rings, their halogen derivatives as well as noble gases and simple inorganic substances follow a single linear dependence of the Gibbs hydrophobic effect energy on their characteristic molecular volume. We can conclude that for all compounds studied, the differences in their structures and shapes do not significantly affect their hydrophobicity. Molecular volume is a main factor determin-

ing the value of $\Delta_{h,e}G^A$. The observed results are in agreement with theoretical conclusions [6] that the Gibbs free energy of cavitation in water is not sensitive to molecular shape.

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