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SOME MODELS FOR EVALUATING THE CAVITY FORMATION ENERGIES IN LIQUIDS

Van Phat Nguyên, B. Gander[1]*, S. Gentili, Elie Sarraf and Nam Trân Ho**

Section de Pharmacie, Institut d'Analyse Pharmaceutique, Université de Lausanne,
CH-1015 Lausanne
[1]Department of Pharmacy, Swiss Federal School of Technology, ETH, Winterthurestrasse 190,
CH-8057 Zürich, Switzerland

Abstract

In the mixing process of solutes into solvents, the cavity formation energy is generally introduced into the energy balance. In this study, models for calculating this type of energy are proposed. These models are based on the Hansen's partial solubility parameters δ_d (MPa$^{1/2}$) dispersive, δ_p (MPa$^{1/2}$) polar and δ_h (MPa$^{1/2}$) hydrogen-bonding, and on the internal pressure P_i (J cm^{-3}) of the solvents.

Keywords: cavity energy, Drago's parameters, interaction energies, solubility parameters

Introduction

Estimation of the internal interaction energies and appreciation of the solvent effects on chemical processes requires the knowledge of the cavity formation energy [1]. Different methods have been suggested in the literature to calculate this type of energy [2–5], but depending on the models used the results obtained are quite disparate and lead to opposite interpretations.

Furthermore, some of the models [6–7] are very complicated to use, because they need several parameters (size and shape of solutes) for numeric applications. Particularly, the work of expansion or contraction is often neglected [8].

For these reasons, we would like to propose a new model for evaluating the cavity formation energy, which is based on the internal pressure and Hansen's partial solubility parameters [9].

Basic considerations and models

According to Dack [10], the presence of a dissolved solute in a solvent affects the structure of the latter. The term structure may refer to the strength of intermo-

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* Author to whom all correspondence should be addressed.

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lecular bonding within a liquid or to the geometry of the molecules of the liquid. In both cases, a dissolved solute must create a cavity in the solvent to accommodate itself. When discussing the strength of structure, two types of interactions, have to be emphasized non-chemical (polar and non-polar) and chemical (hydrogen-bonding). Thus, energies related to non-chemical interactions are of physical nature, expressed by the internal pressure, P_i, and mainly of dispersion type, whereas those related to chemical interactions represent the difference between the cohesive pressure and the internal pressure.

In the cavity formation process the question arises whether the cohesive or the internal pressure is perturbed. In this content, we should take into account that the cohesive pressure is a measure of the total molecular cohesion per unit volume [11], and that on vaporization all intermolecular bonds or interactions are broken. On the other hand, the internal pressure is a measure of the internal energy of a liquid when it undergoes a small isothermal expansion. Such a change in volume does not necessarily disrupt all intermolecular forces. In this situation, the interactions most affected are the dispersion, and dipole forces. Finally, since the cavity formation process is an isothermal expansion [12] occuring in the liquid state, the internal pressure should be the main variable of the cavity formation energy.

According to Bagley [13], the internal pressure is a function of two of Hansen's partial solubility parameters (δ_d=dispersive and δ_p=polar) ($MPa^{1/2}$). Considering also the work of Ramos [14], the following boundary conditions for the cavity formation process can be defined:

(i) All molecules of solvents remain in the liquid state (there is no phase transition), so that the energy is mainly a potential energy.

(ii) The short range molecular order in the liquid is not destroyed, perturbation of polarity and hydrogen-bonding will occur, if the components in the binary mixtures possess a chemical structure available for such perturbation.

(iii) Solvent structure is altered (built up destroyed) in the mixing process.

(iv) Under the aforementioned considerations, solvents may be classified into the three categories of protic solvents, dipolar aprotic solvents (μ>2 D) and solvents of low polarity (μ<2 D) [15]. For these three classes of solvents we propose the following three Eqs (1–3) to determine the cavity formation energy, $\Delta_C E_i$ (kJ mol^{-1}).

In solvents of low polarity (μ<2 D), the cavity formation energy is mainly dispersive:

$$\Delta_C E_i = \overline{V}_i(\delta_{d,j}^2) + P_j(\overline{V}_i - V_i) \tag{1}$$

where $\overline{V}_i$ and V_i (cm^3 mol^{-1}) are the partial molar and the molar volume of the solute respectively.

In polar aprotic solvents (μ>2 D), the cavity formation contains an additional polar orientational force, which depends on the dipole moment μ:

$$\Delta_C E_i = \overline{V}_i\left(\delta_{d,j}^2 + \frac{1}{2}\delta_{p,j}^2\right) + P_j(\overline{V}_i - V_i) \tag{2}$$

Finally in protic solvents, hydrogen-bonding increases the strength of electrostatic effects and creates a geometrical order in these liquids:

$$\Delta_C E_i = \overline{V}_i(\delta^2_{d,j}) + \frac{1}{2}\overline{V}_j(\delta^2_{p,j} + \delta^2_{h,j}) + P_j(\overline{V}_i - V_i) \tag{3}$$

The work of contraction or expansion of solvents results from the product of the solvent internal pressure and the change of the molar volume of the solute $P_j(\overline{V}_i - V_i)$.

The adequacy of these Eqs (1) to (3) for different binary mixtures was examinated by Eqs (4) or (5), an alternative method [1] for evaluating $\Delta_C E_i$.

When the partial molar volume of solute is available:

$$\Delta_C E_i = (\Delta_{mix}Q_p)_i - P_j(\overline{V}_i - V_i) - \Delta_v E_i + 2\overline{V}_i\delta_{d,i}\delta_{d,j} +$$

$$+ 2\overline{V}_i\delta_{p,i}\delta_{p,j} + E_iE_j + C_iC_j \tag{4}$$

where $(\Delta_{mix}Q_p)_1$, $\Delta_v E_i$ are the partial mixing heat at infinite dilution and the vaporization energy of the solute respectively, and E and C are Drago's parameters [16].

When the partial molar volume of solute is not available:

$$\Delta_C E_i = (\Delta_{mix}Q_p)_i - \Delta_v E_i + 2V\delta_{d,i}\delta_{d,j} + 2V\delta_{p,i}\delta_{p,j} + E_iE_j + C_iC_j \tag{5}$$

Table 1 Solvent properties in term of molar volume, V, of dipole moment, μ, of Hansen's three partial solubility parameters, δ_d (dispersive) [17], δ_p (polar) [17] and δ_h (hydrogen-bonding) [17], and of Drago's parameters, E (electrostatic), and C (covalent) [16]

Substance	V [17]/	μ [17]/	δ_d [17]/	δ_p [17]/	δ_h [17]/	E [16]/	C [16]/
	$cm^3\ mol^{-1}$	D	$MPa^{1/2}$	$MPa^{1/2}$	$MPa^{1/2}$	$kJ^{1/2}/mol^{-1/2}$	
Cyclopentane	94.86	0	16.5	3.9	0	0	0
Cyclohexane	108.79	0	16.5	3.1	0	0	0
2-methylpentane	133.02	0	14.4	0	0.8	0	0
3-methylpentane	130.80	0	14.6	0	0	0	0
2,2-dimethylbutane	134.06	0	13.7	0	0	0	0
2,3-dimethylbutane	131.40	0	14.2	0	0	0	0
1-hexene	126.05	0	14.0	0	0	0	0
n-pentane	116.26	0	14.4	0	0	0	0
n-hexane	131.80	0	14.7	0	0	0	0
n-heptane	147.57	0	15.3	0	0	0	0
n-octane	163.61	0	15.4	0	0	0	0
n-nonane	179.94	0	15.6	0	0	0	0
n-decane	196.28	0	15.8	0	0	0	0
n-undecane	212.65	0	16.0	0	0	0	0
n-dodecane	228.89	0	16.2	0	0	0	0
tetra-chloromethane	97.1	0	17.8	0	0.6	0	0

Table 1 Continued

Substance	V [17]/	μ [17]/	δ_d [17]/	δ_p [17]/	δ_h [17]/	E [16]/	C [16]/
	$cm^3\ mol^{-1}$	D	$MPa^{1/2}$	$MPa^{1/2}$	$MPa^{1/2}$	$kJ^{1/2}/mol^{-1/2}$	
Toluene	106.8	0	18.0	1.4	2	0	0
Benzene	89.4	0	18.4	0	2	0	0
tert-butanol	94.8	1.66	14.9	5.1	13.9	2.6	1.27
1-butanol	91.9	1.75	16.0	5.7	15.8	2.6	1.27
iso-propanol**	76.95	1.66	15.8	7.2	16.0	–	–
di-ethyl ether	104.8	1.15*	14.5	2.9	5.10	3.73	3.33
iso-propyl ether	140.0	1.38	13.7	2.1	2.4	3.9	3.39
Butyl ether	170.2	1.18*	14.58	4.29	4.49	3.9	3.41
tri-ethylamine	140.0	0.87	14.6	3.7	1.9	2.7	11.7
di-ethylamine	102.9	1.11	13.39	6.99	6.29	2.49	9.28
Butylamine**	99.59	1.37*	15.6	3.7	7.2	–	–
Pyridine	80.90	2.37	18.97	8.79	5.89	3.64	7.24
Acetonitrile	52.6	3.35	15.27	17.95	6.1	3.35	1.45
Acetone	74.0	2.69*	15.60	12.3	7.0	3.55	2.57
Ethyl acetate	98.5	1.82	13.4	8.6	8.9	3.31	2.00
di-methyl sulfoxide	71.3	4.06	18.4	16.4	10.2	4.9	3.00
Methylethylketone	90.1	2.76	16.0	9.0	5.10	3.41	2.53
N,N dimethylacetamide	92.5	3.71	16.78	11.49	10.18	3.35	1.45
N,N dimethyformamide	77.0	3.24	17.38	13.68	11.28	4.48	2.68

* At 20°C

** E, C are not given in literature, we use the energy's values of formation hydrogen bonding [18].

Materials

For numeric verifications of the proposed models, a serie of compounds was examined, and their properties are given in Table 1.

Results and discussion

For estimating the cavity formation energy according to Eqs (4) or (5) some measured quantities are given in Table 2.

For comparison, the values of the cavity formation energy are either calculated according to the proposed models (Eqs (1–3)) or estimated according to Eqs (4) or (5). Tables 3 –6 give the corresponding energy values and coefficients of variation.

Table 2 Values of the partial molar volume $\overline{V}$, the internal pressure P_i, and the partial heat of mixing $(\Delta_{mix}Q_p)_i$

Solute	Solvent	$\overline{V}$/cm^3 mol^{-1}	P_i/J cm^{-3}	$(\Delta_{mix}Q_p)_i$/kJ mol^{-1}
Cyclopentane [7]	*n*-pentane	–	–	0.26
	n-hexane	–	–	0.29
	n-heptane	–	–	0.32
	n-octane	–	–	0.39
	cyclohexane	–	–	0.13
	n-dodecane	–	–	0.62
Cyclohexane [7]	*n*-hexane	–	–	0.63
	n-heptane	–	–	0.80
	n-octane	–	–	0.90
	n-nonane	–	–	0.97
	n-decane	–	–	0.96
	n-undecane	–	–	0.01
	n-dodecane	–	–	0.73
	cyclopentane	–	–	0.08
	1-hexene	–	–	0.61
2-methylpentane [7]	*n*-pentane	–	–	0.00
	n-hexane	–	–	0.02
	n-heptane	–	–	0.05
	n-octane	–	–	0.08
	n-decane	–	–	0.17
	n-dodecane	–	–	0.16
3-methylpentane [7]	*n*-pentane	–	–	0.00
	n-hexane	–	–	0.01
	n-heptane	–	–	0.04
	n-octane	–	–	0.06
	n-decane	–	–	0.16
	n-dodecane	–	–	0.28
2,2-dimethylbutane [7]	*n*-heptane	–	–	0.08
	n-octane	–	–	0.012
	n-decane	–	–	0.27
	n-dodecane	–	–	0.42
	cyclohexane	–	–	0.59
2,3-dimethylbutane [7]	*n*-pentane	–	–	0.00
	n-hexane	–	–	0.01
	n-heptane	–	–	0.04
	n-octane	–	–	0.07

Table 2 Continued

Solute	Solvent	$\bar{V}$/cm^3 mol^{-1}	P_i/J cm^{-3}	$(\Delta_{mix}Q_p)_i$/kJ mol^{-1}
2,3-dimethylbutane [7]	*n*-decane	–	–	0.18
	n-dodecane	–	–	0.32
di-ethyl ether [7]	*n*-heptane	–	–	2.845
	cyclohexane	–	–	4.100
	CCl_4	–	–	–1.75
	toluene	–	–	–0.41
	benzene	–	–	0.836
	tri-ethylamine	–	–	0.292
	n-butylether	–	–	0.460
	ethyl acetate	–	–	1.171
	DMF	–	–	2.217
	di-methyl sulfoxide	–	–	5.564
	n-octanol	–	–	2.677
	tert-butanol	–	–	2.217
	methanol	–	–	0.251
n-butanol [19]	*n*-heptane	–	–	24.267
	cyclohexane	–	–	24.852
	CCl_4	–	–	19.204
	toluene	–	–	16.945
	benzene	–	–	16.945
	tri-ethylamine	–	–	–4.560
	n-butyl ether	–	–	8.451
	ethyl acetate	–	–	8.744
	DMF	–	–	3.305
	di-methyl sulfoxide	–	–	4.560
	n-octanol	–	–	0.376
	tert-butanol	–	–	–2.301
	methanol	–	–	0.878
n-butanol [18]	*n*-hexane	–	–	23.012
2-butanol [18]	*n*-hexane	–	–	23.012
iso-propanol [18]	*n*-hexane	–	–	24.685
Butylamine [18]	*n*-hexane	–	–	5.313
Butyl ether [18]	*n*-hexane	–	–	0.418
Acetone [18]	*n*-hexane	–	–	9.539
Methylethylketone [18]	*n*-hexane	–	–	7.949
Acetonitrile [18]	*n*-hexane	–	–	14.644
n-butanol [18]	*n*-butyl ether	–	–	5.062

Table 2 Continued

Solute	Solvent	$\bar{V}$/cm^3 mol^{-1}	P_i/J cm^{-3}	$(\Delta_{mix}Q_p)_i$/kJ mol^{-1}
n-butanol [18]	butylamine	–	–	–8.284
	acetone	–	–	7.112
	acetonitrile	–	–	9.414
2-butanol [18]	methyl ethyl ketone	–	–	7.614
iso-propanol [18]	acetone	–	–	7.363
n-butanol]20]	*di*-methyl sulfoxide	–	–	4.100
	DMF	–	–	3.000
tert-butanol [19]	*di*-methyl sulfoxide	–	–	5.000
	DMF	–	–	3.500
tert-butanol [1]	ethyl ether	94.79	0.242	4.857
	iso-propyl ether	94.84	0.231	7.460
tert-butanol [1]	*n*-butyl ether	96.53	0.234	8.573
	acetonitrile	96.63	0.303	9.497
tert-butanol [1]	pyridine	95.16	0.406	2.477
	DMA	95.91	0.322	2.138
tert-butanol [1]	DMF	95.02	0.350	3.171
	tri-ethylamine	91.37	0.239	0.795
	di-ethylamine	89.75	0.215	2.686
Ethyl ether [1]	*tert*-butanol	104.21	0.269	1.487
iso-propyl ether [1]	*tert*-butanol	142.21	0.260	2.920
n-butyl ether [1]	*tert*-butanol	172.00	0.255	4.719
Acetonitrile [1]	*tert*-butanol	54.56	0.303	6.159
Pyridine [1]	*tert*-butanol	81.14	0.279	–0.286
DMA [1]	*tert*-butanol	94.10	0.273	1.448
DMF [1]	*tert*-butanol	78.31	0.281	3.756
tri-ethylamine [1]	*tert*-butanol	136.43	0.260	–2.386
di-ethylamine [1]	*tert*-butanol	99.52	0.269	–4.494

Table 3 Values of cavity formation energy as calculated by the proposed model (Eq. (1)), $\Delta_cE_{calc\,1}$ or as estimated, according to Eq. (5), $\Delta_cE_{est\,5}$

Solute	Solvent	$\Delta_cE_{calc\,1}$/ kJ mol^{-1}	$\Delta_cE_{est\,5}$/ kJ mol^{-1}	*CV*/ %
Cyclopentane	*n*-pentane	18.418	19.669	–6.4
	n-hexane	19.975	21.059	-5.1
	n-heptane	21.603	22.205	–4.4

Table 3 Continued

Solute	Solvent	$\Delta_c E_{calc\ 1}$/ kJ mol^{-1}	$\Delta_c E_{est\ 5}$/ kJ mol^{-1}	CV/ %
Cyclopentane	*n*-octane	21.603	22.496	–4.0
	n-dodecane	24.276	24.894	–2.5
	cyclohexane	25.849	25.825	0.1
Cyclohexane	*n*-hexane	23.416	24.151	–3.0
	n-heptane	25.022	25.465	–1.7
	n-octane	25.481	25.799	–1.2
	n-nonane	26.269	26.474	–0.8
	n-decane	26.977	27.157	–0.7
	n-undecane	26.745	27.849	–4.0
	cyclopentane	28.489	28.198	1.0
	1-hexene	22.916	22.557	1.6
2-methylpentane	*n*-pentane	27.584	27.584	0.0
	n-hexane	29.519	29.532	0.0
	n-heptane	31.082	31.139	–0.2
	n-octane	31.495	31.548	–0.2
	n-decane	33.117	33.208	–0.2
	n-dodecane	34.640	34.911	–0.8
3-methylpentane	*n*-pentane	27.118	27.118	0.0
	n-hexane	29.038	29.039	0.0
	n-heptane	30.595	30.619	–0.1
	n-octane	30.997	31.021	–0.1
	n-decane	32.625	32.653	–0.1
	n-dodecane	34.273	34.328	–1.6
2,2-dimethylbutane	*n*-heptane	31.118	31.381	–0.8
	n-octane	31.418	31.793	–1.2
	n-decane	33.145	33.466	–1.0
	n-dodecane	34.764	35.182	–1.2
	cyclohexane	36.036	36.497	–1.3
2,3-dimethylbutane	*n*-pentane	27.242	27.247	0.0
	n-hexane	29.118	29.172	–0.2
	n-heptane	30.641	30.760	–0.4
	n-octane	31.044	31.163	–0.4
	n-decane	32.646	32.803	–0.5
	n-dodecane	34.279	34.485	–0.6
1-hexene	*n*-hexane	25.958	27.983	–7.2
	cyclohexane	34.311	34.316	0.0

Table 3 Continued

Solute	Solvent	$\Delta_c E_{calc\,1}$/ kJ mol^{-1}	$\Delta_c E_{est\,5}$/ kJ mol^{-1}	*CV*/ %
di-ethyl ether	*n*-heptane	27.351	24.532	11.5
	cyclohexane	33.243	29.227	13.7
	CCl_4	31.669	33.204	–4.6
	toluene	33.880	33.955	–0.2
	benzene	36.217	35.481	2.1
	tri-ethylamine	20.751	22.339	–7.1
	n-butyl ether	21.284	22.339	–4.7
2-butanol	*n*-hexane	19.880	20.406	–2.6
iso-propanol	*n*-hexane	16.628	17.536	–5.2
Butylamine	*n*-hexane	21.520	20.245	6.3
Butyl ether	*n*-hexane	36.735	36.917	–0.5
Acetone	*n*-hexane	15.990	14.760	8.3
Methyl ethyl ketone	*n*-hexane	19.469	17.806	9.3
n-butanol	*n*-hexane	19.858	17.250	15.1
	n-heptane	20.240	21.419	–5.5
	cyclohexane	25.503	25.518	–0.1
	CCl_4	24.858	28.990	–14
	toluene	28.356	29.646	–4.4
	benzene	29.110	30.978	–6.0
	tri-ethylamine	15.100	19.504	–22.6
n-butanol	*n*-butyl ether	21.235	19.504	–8.9
n-butanol	*n*-butyl ether	19.535	20.005	–2.3
n-butanol	butylamine	22.364	23.726	–5.7

Table 4 Values of cavity formation energy as calculated by the proposed model (Eq. (2)), $\Delta_c E_{calc\,2}$ or as estimated, according to Eq. (5), $\Delta_c E_{est\,5}$

Solute	Solvent	$\Delta_c E_{calc\,2}$ / kJ mol^{-1}	$\Delta_c E_{est\,5}$/ kJ mol^{-1}	*CV*/ %
di-ethyl ether	ethyl acetate	20.961	22.693	–7.6
	DMF	37.264	41.564	–10
	di-methyl sulfoxide	45.292	49.574	–8.6
iso-propanol	acetone	24.547	29.050	–15
n-butanol	ethyl acetate	19.275	19.813	–2.7
	DMF	34.753	36.289	–4.2

Table 4 Continued

Solute	Solvent	$\Delta_c E_{calc\,2}$ / kJ mol^{-1}	$\Delta_c E_{est\,5}$/ kJ mol^{-1}	CV/ %
n-butanol	*di*-methyl sulfoxide	43.283	43.283	0.0
	acetone	29.316	32.401	–9.5
	acetonitrile	36.400	34.687	4.9
tert-butanol	*di*-methyl sulfoxide	45.924	44.844	2.4
	DMF	37.036	37.552	-1.4

Table 5 Values of cavity formation energy as calculated by the proposed model (Eq. (2)), $\Delta_c E_{calc\,2}$ or as estimated, according to Eq. (4), $\Delta_c E_{est\,4}$

Solute	Solvent	$\Delta_c E_{calc\,2}$ / kJ mol^{-1}	$\Delta_c E_{est\,4}$/ kJ mol^{-1}	CV/ %
tert-butanol	pyridine	38.050	39.092	–2.7
	DMA	33.682	32.754	2.8
	DMF	37.630	36.210	3.9
	acetonitrile	38.665	37.173	4.0

Table 6 Values of cavity formation energy as calculated by the proposed model (Eq. (3)), $\Delta_c E_{calc\,3}$ or as estimated, according to Eq. (4), $\Delta_c E_{est\,4}$

Solute	Solvent	$\Delta_c E_{calc\,3}$ / kJ mol^{-1}	$\Delta_c E_{est\,4}$/ kJ mol^{-1}	CV/ %
di-ethyl ether	*tert*-butanol	39.357	37.888	3.9
iso-propyl ether	*tert*-butanol	51.023	51.740	-1.3
n-butyl ether	*tert*-butanol	60.289	62.535	–3.6
Acetonitrile	*tert*-butanol	20.668	19.836	4.2
Pyridine	*tert*-butanol	34.958	29.500	18.5
DMA	*tert*-butanol	29.215	34.212	–14.6
DMF	*tert*-butanol	24.201	28.471	–14.9
tri-ethylamine	*tert*-butanol	55.426	49.602	11.7
di-ethylamine	*tert*-butanol	36.290	36.183	0.3

From these tables, an excellent correspondence becomes evident between the cavity formation energy values calculated by the proposed models as compared to those obtained from an alternative method. Some divergences, however, occur for mixtures of solutes and solvents of high polarity or interacting through hydrogen-

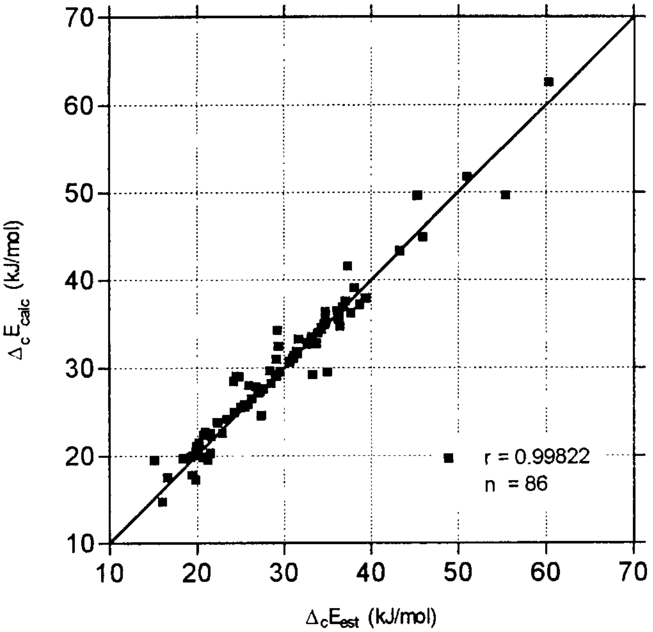

Fig. 1 Correlationship between $\Delta_c E_{calc}$ and $\Delta_c E_{est}$

bonding. For the time being, we do not known if these divergences result from the values of Drago's parameters. The validity of the proposed models to calculate $\Delta_c E_i$ is illustrated in Fig. 1. From this linear fit between $\Delta_c E_{calc}$ (Eqs (1) or (2) or (3)) and $\Delta_c E_{est}$ (Eqs (4) or (5)) a good correlation coefficient (r=0.9960) is obtained.

Conclusion

The good agreement between the $\Delta_c E_{cal}$ and $\Delta_c E_{est}$ values allows the following conclusions:

– In the mixing process, the hypothesis of the formation of a cavity or the perturbation of solvent structure cannot be rejected for maintaining the energy balance of the interaction model.

– The energy used in this process is mainly dispersive and represents a component of the internal pressure. This energy can be calculated from the molecular properties of solvents and solute without further experimental measurements. A possibility which is of great practical interest.

– The proposed models for calculating the cavity formation energy are very simple to use and seem to describe well the cavity process.

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