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STATISTICAL STUDY OF THE DISSOCIATION AND SOLVATION PROCESSES FOR DICHLORO-SUBSTITUTED BENZOIC ACIDS: ADDITIVE AND STERIC EFFECTS

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ABSTRACT

The influence of chlorine atoms on the ionization and solvation processes for 2,6- and 3,5-chloro disubstituted benzoic derivatives was studied from the statistical viewpoint

This study was carried out by comparing the enthalpy values of these processes with those of the corresponding monosubstituted chloro derivatives in water–DMSO mixtures over the mole fraction range 0–0 8 For this purpose, a monoparametric regression analysis was used In this analysis, total standard deviation, slope and intercept standard deviations, correlation coefficient and the Student *t*-test of the enthalpy values were taken into account

The additive principle for both compounds and steric effect for the 2,6-dichloro derivative were also studied

INTRODUCTION

The behaviour of the dissociation and solvation processes of ions and undissociated molecules has been systematically studied in our laboratory [1–7] This study has been carried out, from the statistical viewpoint, by using mono- and diparametric regression analyses, in order to ascertain in which benzene ring positions the influence of the substituent groups plays a major role Indeed, the statistical analysis is able to supply useful methods for revealing small variations of structure in the skeleton of the molecule due to the introduction of the same groups in different positions or of different groups in the same positions [8–13]

This work aims to study the influence of the chlorine atom in positions 2, 3, 5 and 6, and compares these effects with those of dihydroxy and dinitro derivatives previously studied [1,2]

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The 2,6-dichloro and 3,5-dichloro acids are compared with the respective 2-chloro and 3-chloro monosubstituted compounds For this purpose, correlations between ionization, molecule and ion solvation processes of mono- and disubstituted chloro derivatives are critically examined

In this way, it is possible to ascertain in which of the two solvation processess the additive effect is prevailing

EXPERIMENTAL AND PROCEDURE

The calorimetric measurements were performed by means of a Tronac 450 calorimeter and a L K B 8700 reaction and solution calorimeter

The calorimetric measurements were processed by means of a BASIC program used on an Olivetti M24 computer [14,15] DMSO (Erba, RP) was purified according to the procedure of Synnot and Butler [16] DMSO–water mixtures were prepared by weighing purified DMSO and CO_2-free, bidistilled water The mole fraction of DMSO in these mixtures ranged from 0 0 to 0 8 Aqueous solutions of 0 099 M NaOH and of 0 99 M HCl in various DMSO–water mixtures were prepared from standard solutions, and their concentrations were checked by potentiometric titrations

The 2,6-dichloro and 3,5-dichlorobenzoic acids (Fluka) were purified by crystallization from water–ether mixtures and their m p checked before use The chloro sodium salts were prepared by adding a NaOH solution of known molarity to 2,6- and 3,5-dichlorobenzoic acids dissolved in the DMSO–water mixtures As a result, 100 g of DMSO–water solution at X mole fraction were obtained

The concentrations of the sodium salts were always in the range 2×10^{-3}–4×10^{-3} M A certain amount of acid (about 4–5% of the original content) was not converted into the salt and remained as free acid to avoid the presence of free alkali

The ionization process of $Y,Z(Cl)_2PhCOOH$ (where the Y,Z are the number pairs 2,6 or 3,5) in the various H_2O–DMSO mixtures can be represented as

$$[Y,Z(Cl)_2PhCOOH]_X \rightarrow [Y,Z(Cl)_2PhCOO^-]_X + (H^+)_X \qquad (1)$$

The partial molar enthalpy of ionization $\Delta\overline{H}_1$ of $Y,Z(Cl)_2PhCOOH$ was obtained by experimental measurements of (a) the partial molar enthalpy of reaction $\Delta\overline{H}_2$ of $Y,Z(Cl)_2PhCOONa$ dissolved in the mixed solvent of X mole fraction, with 0 99 M HCl also dissolved in X mole fraction

$$\begin{aligned}&[Y,Z(Cl)_2PhCOO^-]_X + (Na^+)_X + (H^+)_X + (Cl^-)_X\\&\quad = [Y,Z(Cl)_2PhCOOH]_X + (Na^+)_X + (Cl^-)_X \qquad (2)\end{aligned}$$

and (b) the partial molar enthalpy of dilution $\Delta\overline{H}_3$ of the same amount of 0 99 M HCl (dissolved in X mole fraction)

$$(\mathrm{H}^+)_X + (\mathrm{Cl}^-)_X = (\mathrm{H}^+)_X + (\mathrm{Cl}^-)_X \qquad (3)$$

The partial molar enthalpy of process (1) can be obtained by subtracting $\Delta\overline{H}_2$ from $\Delta\overline{H}_3$ For each of the water–DMSO mixtures at X mole fraction, $\Delta\overline{H}_1$ refers to the ionization process of 1 mol of $Y,Z(\mathrm{Cl})_2\mathrm{PhCOOH}$ dissolved at infinite dilution in 1000 g of mixed solvent, yielding 1 mol of protons and 1 mol of $Y,Z(\mathrm{Cl})_2\mathrm{PhCOO}^-$ ions solvated in the same amount of solvent

In order to refer process (1) to an initial thermodynamic state only, the solution enthalpies of crystalline $Y,Z(\mathrm{Cl})_2\mathrm{PhCOOH}$ $\Delta\overline{H}_s$ in the various solvent mixtures were measured

$$Y,Z(\mathrm{Cl})_2\mathrm{PhCOOH}_{(\mathrm{cry})} \rightarrow [Y,Z(\mathrm{Cl})_2\mathrm{PhCOOH}]_X \qquad (4)$$

so that ΔH_5 $(= \Delta H_1 + \Delta H_4)$ values obtained for the process

$$Y,Z(\mathrm{Cl})_2\mathrm{PhCOOH}_{(\mathrm{cry})} \rightarrow [Y,Z(\mathrm{Cl})_2\mathrm{PhCOO}^-]_X + (\mathrm{H}^+)_X \qquad (5)$$

refer to an identical initial thermodynamic state In processes (2) and (4), concentrations ranging from 2×10^{-3} to 4×10^{-3} M were used Therefore, the $\Delta\overline{H}$ values related to these processes were assumed to be equal to $\Delta H^{\ominus}$ values [17]

A program which processes data using the monoparametric linear regression equation, with total standard deviation, slope and intercept standard deviations and correlation coefficients was run on an Olivetti M24 computer using the above enthalpy values For this monoparametric regression equation the following null hypotheses were considered (1) $b = 0$, (2) $b = 0$ 5, (3) $b = 1$, (4) $b = 2$ The null hypotheses were tested by using the Student t-test The t values of b were calculated by means of the expression $t = (b - B)/S_b$ (where $B = 0$, 0 5, 1, 2, S_b is the standard deviation of b) and were compared with values from standard t-tables If $t > t_{\mathrm{C\,L}\;n-2}$, where $n - 2$ is the degree of freedom of the system and C L the confidence level for the significance of the regression, then for C L < 0 95 the null hypothesis is accepted (chemical hypothesis), while for C L > 0 999 its rejection is highly significant

RESULTS AND DISCUSSION

Tables 1 and 2 show $\Delta H_1^{\ominus}$ values of processes (1), (4) and (5) for the 2,6- and 3,5-dichlorosubstituted benzoic acids For the sake of comparison, it is convenient to express the ionization enthalpy values $\Delta H_1^{\ominus}$ as the difference between the values obtained in the mixed solvent at X mole fraction and those in pure water, so that

$$\delta\Delta H_1 = (\Delta H_1^{\ominus})_X - (\Delta H_1^{\ominus})_{X=0}$$

TABLE 1

Enthalpy values (kcal mol^{-1}) of processes (1), (4) and (5) for 2,4-dichlorobenzoic acid in water–DMSO mixtures of various mole fractions at 25 °C

X(DMSO)	$\Delta H_1^\ominus$	$\Delta H_4^\ominus$	$\Delta H_5^\ominus$
0 0	−0 66	−0 80	−1 46
0 1	−1 53	2 59	1 06
0 2	−1 06	3 26	2 20
0 3	−0 51	2 25	1 74
0 4	0 50	0 99	1 49
0 5	1 37	−0 12	1 25
0 6	2 08	−0 82	1 26
0 7	3 13	−1 06	2 07
0 8	4 33	−2 03	2 30

These values are relative to the transfer of the ionization process, while $\delta\Delta H_4^\ominus$ and $\delta\Delta H_5^\ominus$ values represent the transfer enthalpy of the undissociated molecules and of the two ions H^+ and $Y,Z(Cl)_2PhCOO^-$, respectively, from pure water to mixed solvent $\delta\Delta H_4^\ominus$ and $\delta\Delta H_5^\ominus$ represent solvation of the molecule and the ions at the various mole fractions, with respect to pure water (Figs 1 and 2) The $\delta\Delta H_1^\ominus$ term, as shown in Fig 1, is favourable to process (1), with respect to that occurring in water, up to $X_{DMSO} = 0\ 3$ Beyond this mole fraction the opposite is true This is due to the inversion, at $X_{DMSO} = 0\ 3$, of the anion solvation with respect to that of the undissociated molecule

As regards the 3,5-dichlorosubstituted species (Fig 2), the ionization process, in the whole mole fraction range, is always favoured, with respect to that occurring in pure water This is again due to the greater solvation of the ion with respect to that of the undissociated molecule

TABLE 2

Enthalpy values (kcal mol^{-1}) of processes (1), (4) and (5) for 3,5-dichlorobenzoic acid in water–DMSO mixtures of various mole fractions at 25 °C

X(DMSO)	$\Delta H_1^\ominus$	$\Delta H_4^\ominus$	$\Delta H_5^\ominus$
0 0	4 43	−0 32	4 11
0 1	2 40	7 08	9 48
0 2	0 75	7 42	8 17
0 3	1 14	7 17	8 31
0 4	2 08	5 77	7 85
0 5	2 75	4 42	7 17
0 6	3 61	3 64	7 25
0 7	4 23	3 03	7 26
0 8	5 42	2 69	8 11

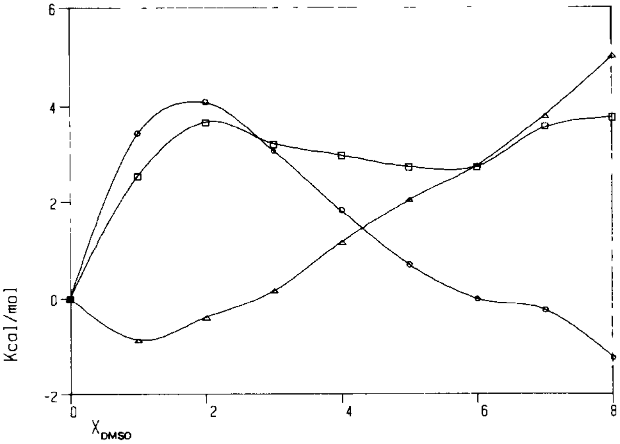

Fig 1 Enthalpy transfer of the ionization process $\delta\Delta H_1^{\ominus}$ (△) and transfer enthalpies of the undissociated molecules $\delta\Delta H_4^{\ominus}$ (○) and their anions $\delta\Delta H_5^{\ominus}$ (□) of the 2,6-dichloro benzoic acid in water–DMSO mixtures

A comparison between the couples of the dissociation, molecule and ion solvation processes of the dichlorosubstituted compounds (Fig 3), shows that the different solvation enthalpies of the ions play a major role in the differentiation of the acidity between the 2,6-dichloro and 3,5-dichloro-benzoic acids The order based on the ionization enthalpies is $2,6(Cl)_2PhCOOH > 3,5(Cl)_2PhCOOH$ For the undissociated molecule solvation, it can be inferred that $2,6(Cl)_2PhCOOH > 3,5(Cl)_2PhCOOH$ For the ions, the scale of solvation shows the following order, $2,6(Cl)_2PhCOO^- > 3,5(Cl)_2PhCOO^-$

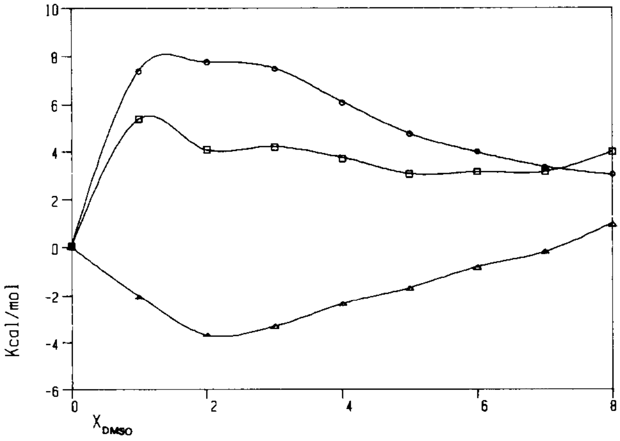

Fig 2 Enthalpy transfer of the ionization process $\delta\Delta H_1^{\ominus}$ (△) and transfer enthalpies of the undissociated molecules $\delta\Delta H_4^{\ominus}$ (○) and their anions $\delta\Delta H_5^{\ominus}$ (□) of the 3,5-dichlorobenzoic acid in water–DMSO mixtures

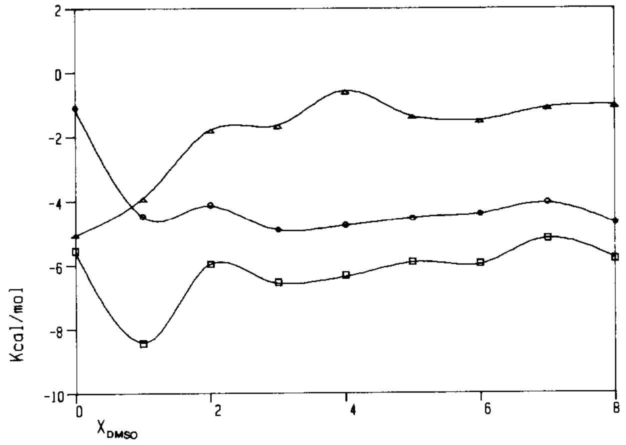

Fig 3 Differences in the enthalpy of ionization ($\Delta H^{\ominus}_{i[2,6(Cl)_2PhCOOH]} - \Delta H^{\ominus}_{i[3,5(Cl)_2PhCOOH]}$ (△) and in enthalpy of solvation between undissociated molecule couples $\Delta H_{[2\,6(Cl)_2PhCOOH]-[3\,5(Cl)_2PhCOOH]}$ (○) and the ion couples $\Delta H_{[2,6(Cl)_2PhCOO^-]-[3\,5(Cl)_2PhCOO^-]}$ (□) of the 2,6-dichloro- and 3,5-dichlorobenzoic acids in various DMSO–water mixtures

The larger solvation of the 2,6-dichloro anion with respect to the 3,5-dichloro one, in the whole mole fraction range, can be ascribed to the fact that chlorine atoms in positions 2 and 6 stabilize the anion by means of charge delocalization due to the two internal bonds (between chlorine atoms and carboxylate group), with a consequent cyclic form of the *ortho*-anion

2,6-Dichlorobenzoic acid also shows a steric effect as a function of the mole fraction variation As the DMSO percentage increases, the anion solvation decreases (Fig 1), reaching a minimum value at $X = 0\ 2$ Beyond this mole fraction the minimum value becomes constant The presence of two methyl groups in the DMSO molecule sterically hinders the cyclic form of the 2,6-chloro anion

For the 2,6-dichlorobenzoic undissociated molecule, it can also be hypothesized that a cyclic form, with a consequent dipole, which in turn stabilizes the charge and makes the molecule more easily solvated than the 3,5-undissociated one

The anion solvation processes play a major role in the ionization processes for both the dichlorosubstituted compounds This opposes the hypothesis that the solvation of the undissociated molecules is the key factor of the ionization processes for the disubstituted compounds [1–7] A monoparametric linear regression analysis, applied to 2,6-, 3,5- and 2- and 3-chloroderivatives could give a satisfactory statistical answer Indeed, as previously shown, statistical analysis presents a useful method for comparing and explaining the substituent effects in the benzene ring in terms of probability Using, for example, a linear monoparametric regression between the enthalpy values of 2,6-dichloro and 2-chloro derivatives, for the ionization and

TABLE 3

Results of monoparametric regression analysis of ionization process for 2,6-dichlorobenzoic acid as a function of the 2-chloroderivative ionization processes

	$\Delta H^{\ominus}_{2,6}$ versus $\Delta H^{\ominus}_{2}$
n	8
Intercept	−1 52
Slope	0 40
S D of intercept	0 55
S D of slope	0 06
S D of regression	0 76
r	0 94
n h slope = 0	C L > 0 999
n h slope = 0 5	C L < 0 95
n h slope = 1	C L > 0 999
n h slope = 2	C L > 0 999

Key n, number of points, S D , standard deviation, r, correlation coefficient, n h , null hypothesis, C L , confidence level

solvation processes, one obtains the equation $y = a + bx$ where, $y = \Delta H_{2,6}$, $x = \Delta H_2$, a is the intercept and b the slope, the b value is related to the so-called "additive principle"

2,6-Dichloro derivative versus 2-chloro derivative

Ionization process

The linear regression equation is highly significant (Table 3)

The null hypothesis (n.h.) $b = 0\ 5$ shows that the coefficient value does not significantly differ from 0 5 The disubstituted derivatives show values

TABLE 4

Results of monoparametric regression analysis of undissociated molecule solvation for 2,6-dichlorobenzoic acid as a function of the 2-chlorobenzoic derivative molecule solvation process

	$\Delta H^{\ominus}_{2,6}$ versus $\Delta H^{\ominus}_{2}$
n	8
Intercept	4 17
Slope	1 08
S D of intercept	0 34
S D of slope	0 11
S D of regression	0 52
r	0 97
n h slope = 0	C L > 0 999
n h slope = 0 5	0 99 < C L < 0 999
n h slope = 1	C L < 0 95
n h slope = 2	C L > 0 999

See Table 3 for key

TABLE 5

Results of monoparametric regression analysis of ion solvation process for 2,6-dichlorobenzoic acid as a function of the 2-chlorobenzoic derivative ions solvation process

	$\Delta H_{2\,6}^{\ominus}$ versus $\Delta H_{2}^{\ominus}$
n	8
Intercept	2 58
Slope	0 10
S D of intercept	0 26
S D of slope	0 04
S D of regression	0 36
r	0 72
n h slope = 0	0 95 < C L < 0 99
n h slope = 0 5	C L > 0 999
n h slope = 1	C L > 0 999
n h slope = 2	C L > 0 999

See Table 3 for key

halved with respect to those of the monosubstituted ones The additive principle is inverted

Solvation process of undissociated molecules

The regression equation is highly significant (Table 4) The *b* value does not significantly differ from 1, so the enthalpic term displays the same statistical weight for the mono- and disubstituted compounds The additive principle is violated

TABLE 6

Results of monoparametric regression analysis of ionization process for 3,5-dichlorobenzoic acid as a function of the 3-chlorobenzoic derivative ionization process

	$\Delta H_{3\,5}^{\ominus}$ versus $\Delta H_{3}^{\ominus}$
n	8
Intercept	− 3 44
Slope	0 36
S D of Intercept	0 56
S D of slope	0 09
S D of regression	0 89
r	0 85
n h slope = 0	0 99 < C L < 0 999
n h slope = 0 5	C L < 0 95
n h slope = 1	C L > 0 999
n h slope = 2	C L > 0 999

See Table 3 for key

TABLE 7

Results of monoparametric regression analysis of undissociated molecules solvation for 3,5-dichlorobenzoic acid as a function of the 3-chlorobenzoic derivative molecules solvation process

	$\Delta H_{3,5}^{\ominus}$ versus $\Delta H_{3}^{\ominus}$
n	8
Intercept	7.57
Slope	1.25
S.D. of intercept	0.25
S.D. of slope	0.11
S.D. of regression	0.45
r	0.98
n.h. slope = 0	C.L. > 0.999
n.h. slope = 0.5	C.L. > 0.999
n.h. slope = 1	C.L. < 0.95
n.h. slope = 2	C.L. > 0.999

See Table 3 for key

Solvation process of ions

Linear monoparametric regression is uncertain (Table 5). The *b* value (0.1) shows that the contribution to the additive principle is negligible.

3,5-Dichlorosubstituted derivative versus 3-chloro derivative

Ionization process

The linear regression is significant (Table 6). The value of *b* is not significantly different from 0.5. The enthalpic term of the disubstituted compound is again halved with respect to that of the monosubstituted one.

TABLE 8

Results of monoparametric regression analysis of ion solvation process for 3,5-dichlorobenzoic acid as a function of the 3-chlorobenzoic derivative ion solvation process

	$\Delta H_{3,5}^{\ominus}$ versus $\Delta H_{3}^{\ominus}$
n	8
Intercept	4.27
Slope	−0.13
S.D. of intercept	0.49
S.D. of slope	0.13
S.D. of regression	0.76
r	0.39
n.h. slope = 0	C.L. < 0.95
n.h. slope = 0.5	0.95 < C.L. < 0.99
n.h. slope = 1	C.L. > 0.999
n.h. slope = 2	C.L. > 0.999

See Table 3 for key

TABLE 9

Results of monoparametric regression analysis of ionization process for 3,5-dichlorobenzoic acid as a function of the 3,5-dinitrobenzoic derivative ionization process

	$\Delta H^{\ominus}_{3,5}$ versus $\Delta H^{\ominus}_{3,5}$
n	7
Intercept	2 60
Slope	0 54
S D of intercept	0 53
S D of slope	0 09
S D of regression	0 62
r	0 94
n h slope = 0	0 99 < C L < 0 999
n h slope = 0 5	C L < 0 95
n h slope = 1	0 99 < C L < 0 999
n h slope = 2	C L > 0 999

See Table 3 for key

Molecule solvation process

The linear regression is highly significant (Table 7) The coefficient *b* does not significantly differ from 1

Ion solvation process

The linear regression is insignificant (Table 8) The value of *b* does not significantly differ from 0 The contribution to the additive principle is nil From this evidence it can be inferred that the molecule solvation process is the prevailing factor in the ionization process, in accordance with the

TABLE 10

Results of monoparametric regression analysis of undissociated molecules solvation process of 3,5-dichlorobenzoic acid as a function of the 3,5-dinitro derivative molecule solvation process

	$\Delta H^{\ominus}_{3,5}$ versus $\Delta H^{\ominus}_{3,5}$
n	7
Intercept	−0 08
Slope	0 96
S D of intercept	0 13
S D of slope	0 05
S D of regression	0 22
r	0 99
n h slope = 0	C L > 0 999
n h slope = 0 5	C L > 0 999
n h slope = 1	C L < 0 95
n h slope = 2	C L > 0 999

See Table 3 for key

TABLE 11

Results of monoparametric regression analysis of ion solvation process of 3,5-dichlorobenzoic acid as a function of the 3,5-dinitroderivative ions solvation process

	$\Delta H^{\ominus}_{3,5}$ versus $\Delta H^{\ominus}_{3,5}$
n	7
Intercept	−0 91
Slope	−0 23
S D of intercept	0 58
S D of slope	0 16
S D of regression	0 45
r	0 56
n h slope = 0	C L < 0 95
n h slope = 0 5	0 99 < C L < 0 999
n h slope = 1	C L > 0 999
n h slope = 2	C L > 0 999

See Table 3 for key

general behaviour of the disubstituted derivatives The additive principle fails mostly because of the nil contribution of the ions

A comparison between the dichloro substituted derivatives with disubstituted derivatives which bear different groups in the same positions can give a deeper insight into the ionization processes

3,5-Dichloro derivative versus 3,5-dinitro derivative

Ionization process

The linear regression is significant (Table 9) The coefficient value (0.54) shows that the $-NO_2$ groups in positions 3 and 5 halve the ΔH values of ionization process with respect to those of the 3,5-dichloro derivatives.

TABLE 12

Results of monoparametric regression analysis of ionization process for 2,6-dichlorobenzoic acid as a function of 2,6-dihydroxy derivative ionization process

	$\Delta H^{\ominus}_{2,6}$ versus $\Delta H^{\ominus}_{2,6}$
n	8
Intercept	3 35
Slope	14 00
S D of intercept	0 89
S D of slope	5 84
S D of regression	1 60
r	0 70
n h slope = 0	C L < 0 95
n h slope = 0 5	C L < 0 95
n h slope = 1	C L < 0 95
n h slope = 2	C L < 0 95

See Table 3 for key

TABLE 13

Results of monoparametric regression analysis of ion solvation process of 2,6-dichlorobenzoic acid as a function of the 2,6-dihydroxy derivative ion solvation process

	$\Delta H^{\ominus}_{2,6}$ versus $\Delta H^{\ominus}_{2,6}$
n	8
Intercept	3 01
Slope	0 02
S D of intercept	0 36
S D of slope	0 06
S D of regression	0 51
r	0 15
n h slope = 0	C L < 0 95
n h slope = 0 5	C L > 0 999
n h slope = 1	C L > 0 999
n h slope = 2	C L > 0 999

See Table 3 for key

Molecule solvation process

The linear monoparametric regression is highly significant (Table 10) The *b* value (which does not significantly differ from 1) signifies that there is the same substituent effects for the chlorine atom and the $-NO_2$ group

Ions solvation process

The linear regression is insignificant (Table 11) again in the ion solvation process no relationship is found Finally, a comparison between 2,6-dichloro and 2,6-dihydroxy derivatives shows that the monoparametric equations for

TABLE 14

Results of monoparametric regression analysis of undissociated molecules solvation process of 2,6-dichlorobenzoic acid as a function of the 2,6-dihydroxy derivative molecules solvation process

	$\Delta H^{\ominus}_{2,6}$ versus $\Delta H^{\ominus}_{2,6}$
n	8
Intercept	4 24
Slope	0 57
S D of intercept	0 56
S D of slope	0 10
S D of regression	0 81
r	0 92
n h slope = 0	0 99 < C L < 0 999
n h slope = 0 5	C L < 0 95
n h slope = 1	0 99 < C L < 0 999
n h slope = 2	C L > 0 999

See Table 3 for key

dissociation (Table 12) and ions solvation (Table 13) are insignificant, while that for the undissociated molecule solvation (Table 14) is significant

This can be explained by considering the intermolecular hydrogen bonds in the *ortho*-hydroxy anion, which makes the 2,6-dihydroxy compound different from all the hydroxy disubstituted derivatives [1,5]

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