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An approach to estimate the energy of the intramolecular hydrogen bond

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Abstract

The problem of the energy of the intramolecular hydrogen bond is widely discussed in the literature, but it has not found an unequivocal univocal solution yet. The partition of the energy of the intramolecular hydrogen bond (ΔE_T) in chloro-derivatives of 2-(*N*-dimethylaminomethyl)-phenols calculated by ab initio and DFT methods was proposed and ‘pure’ ΔE_T values were estimated. These values correlate well with those of $r(\text{H} \cdots \text{N})$ and electron density $\rho(r)$ obtained by the AIM method. © 2002 Elsevier Science B.V. All rights reserved.

1. Introduction

An increasing interest in intramolecular hydrogen bonds has been revealed in recent years [1–11], because of the interesting behavior both from the practical and theoretical points of view. Their enhanced stability, in comparison with an intermolecular complex of the same energy [12], makes them a very interesting model system in the study of the influence of surroundings [13] and substitution [14] on the properties of the hydrogen bond, especially for the modification of the potential for proton movement within the hydrogen bridge [15]. Because of this stability, neither the compositions nor structures of these compounds

change seriously when the temperature or solvent are varied [12,13,16]. Some compounds with intramolecular hydrogen bonds (so-called resonance-assisted hydrogen bonds [17]) can be potentially applied in practice as molecular switches, elements of molecular memory or fluorescence probes in biological systems [18–20].

There are, however, specific features of such hydrogen bonds, such as transfer of interactions between acid–base centers within the molecule [3], the effects of hydrogen bridge bending, diminishing of the acid–base interactions [21] and, as a consequence of this, the decrease of the $\nu(\text{OH})$ band shift and its intensity [14].

The principal question concerning the energy of the hydrogen bond cannot be solved here unambiguously [7–9]. The formation of a chelate ring is concerned not only with acid–base interactions, but also with pronounced geometric and electronic

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structure changes in the system [22,23]. When the reference state in intermolecular interactions is the system of components at a large distance from each other, in intramolecular complexes one of the conformers with a broken intramolecular hydrogen bond is taken as the reference state [7,8,10]. It seems that there are at least three such forms [cf. Scheme 1] [1,9] with a hydroxy group (II) rotated away, with a group such as the dialkylaminomethyl group in ortho-(*N*-dialkylaminomethyl)-phenols rotated out the basic component of the system (III), or a completely ‘open’ conformation (IV), where both groups are rotated (double rotated in the nomenclature of Scheiner [1]). The most popular assumption is to take as a reference the state with a hydrogen bond broken by the hydroxy group rotation [7,8,10]. The value of estimated energy of the hydrogen bond strongly depends on the choice of this reference state [7–9]. The aim of this work is to study the differences in energy between all these four conformers in order to understand which components of the interactions are included in the particular ‘energies of the hydrogen bond’. For these reasons we have selected five molecules with increasing amounts of chlorine substitutes in the phenol ring – 2-(*N*-dimethylaminomethyl)-4-chlorophenol (**1a**), 2-(*N*-dimethylaminomethyl)-6-chlorophenol (**1b**), 2-(*N*-dimethylaminomethyl)-5,6-dichlorophenol (**2a**), 2-(*N*-dimethylaminomethyl)-4,6-dichlorophenol (**2b**), 2-(*N*-dimethyloaminomethyl)-4,5,6-trichlorophenol (**3**), as well as unsubstituted 2-(*N*-dimethyl-

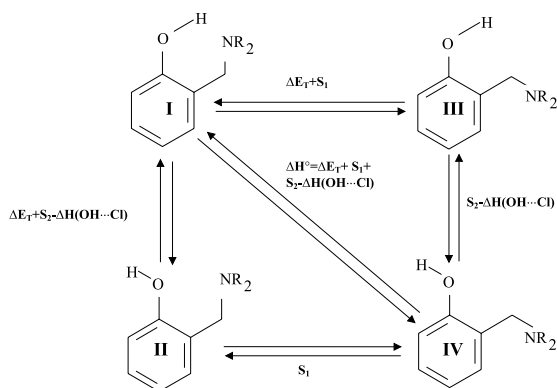
aminomethyl)-phenol (**0**) (DMAP), with the aim to study the change of the content of different kinds of interactions as a function of increasing number of chlorine substituents, i.e., the strength of hydrogen bonding. For this purpose we have used three, medium advanced, quantum chemical methods which seem to be sufficient to describe the basic structural properties of molecules of DMAP type. They are the B3LYP/6-31G**, MP2/6-31G** and B3LYP/d95** methods as included in the GAUSSIAN 98 program [24]. The AIM [25] analysis has been performed with the AIM2000 code [26], with all default options.

We analyzed the energy differences between particular conformers with the help of a kind of thermodynamic cycle, presented in Scheme 1.

ΔE_T , the ‘pure’ energy of the intramolecular hydrogen bonding shown in Scheme 1, has a character of hydrogen bonding interactions analogous to that in intermolecular systems, while S_1 and S_2 result from interactions of dimethyloaminomethyl and hydroxy groups with the rest of the chelate ring, respectively. $\Delta H(\text{OH} \cdots \text{Cl})$ is the energy of the intramolecular hydrogen bond of $\text{OH} \cdots \text{Cl}$ type in II and IV. Such a partition of the energy of interactions done by quantum mechanical calculations is arbitrary, but gives some insight into the character of the intramolecular interactions which we are going to analyze as a function of increasing number of substituted chlorine atoms in DMAP.

Within such an approach the energy difference between states I and II describes the intramolecular interactions of the hydrogen bonding character plus some structural relaxation resulting from the hydroxy group rotation out. Defined in this way, the energy of the hydrogen bond $\Delta E_{\text{HB}} = E_{\text{II}} - E_{\text{I}}$ still contains the steric repulsion between the oxygen and nitrogen atoms within the chelate ring. The corrections on the intramolecular hydrogen bond of $\text{OH} \cdots \text{Cl}$ type are necessary for compounds substituted by a chlorine atom in the ortho position and they are based on calculations for related chlorophenols in the ‘open’ and hydrogen bonded forms.

The above-defined energy of the hydrogen bond ΔE_T can be called ‘theoretical’, because it describes ‘pure’ acid–base hydrogen bonding. On the other hand, the ‘thermodynamic’ value of ΔH^0 of the



Scheme 1. Thermodynamic cycle describing the partition of the energy of intramolecular hydrogen bond.

formation of intramolecular hydrogen bonding, potentially measurable if the open states are available, should be related to the lowest energetic state, IV. The IV state should be lower energetically than III because of the lack of steric repulsion (S_2) between the hydroxy and methine groups. The energy difference between these states can be used for an estimation of (S_2), if the 6-chlorine substituent does not occur in a compound. Otherwise, the $\Delta H(\text{OH} \cdots \text{Cl})$ value should be estimated from independent calculations on phenols, as was stated above.

The difference of energy $E_{\text{II}} - E_{\text{IV}}$ (S_1) is an approximation of the steric interaction of the NR_2 group with other heavy atoms forming the chelate ring.

Taking into consideration the thermodynamic cycle presented in Scheme 3, we estimated the energies of S_1 , S_2 , and the $\text{O}-\text{H} \cdots \text{Cl}$ interactions and, finally, the ‘theoretical’ energy (ΔE_{T}) value of the intramolecular hydrogen bonding.

2. Results and discussion

2.1. The thermodynamic cycle approach

In this approach we do not use the results of the calculations on phenols to avoid the differences between $\Delta H(\text{OH} \cdots \text{Cl})$ in phenols and Mannich bases. The results of the energy calculations of the four conformers of chloro-substituted Mannich bases are presented in Table 1 as energy differences between particular states.

The energy values obtained by the B3LYP/6-32G**, MP2/6-31G** and B3LYP/d95** meth-

ods are shown as A, B, C-type results, respectively. The reliability of calculations can be verified by comparing the energy of direct transfer between particular forms, IV to I for example, and by an indirect way, IV–II–I or IV–III–I. All presented results were tested and, within the particular quantum mechanical methods, the agreement in calculations was very good. All these values will be applied further as basic data in an estimation of the thermodynamic characteristics of the hydrogen bond.

The energy differences between states IV and I are, by definition, equal to ΔH^0 (see Scheme 3) and presented in Table 2. For compounds **1b**, **2a**, **2b** and **3**, the additional interaction to the *o*-chlorine atom changes the energy of state IV and the thermodynamic values of ΔH^0 cannot be used directly for comparison in the whole series of compounds. One can define the value of $\Delta H(\text{O}-\text{H} \cdots \text{N})$, which describes the interaction within the intramolecular hydrogen bonding after corrections in the energy of the open form IV on interactions of the $\text{OH} \cdots \text{Cl}$ -type hydrogen bond ($\Delta H(\text{O}-\text{H} \cdots \text{Cl})$). In such a way the energy of form I will be related to the uniform state IV with corrected energy. $\Delta H(\text{O}-\text{H} \cdots \text{N})$ can be used for comparison between different compounds, and it can be taken as a crude measure of the hydrogen bond energy.

If S_1 and S_2 do not depend on the position of substitution of the chlorine atoms in the phenol ring, the scales of hydrogen bond energy related to the II, III or IV states, as well as the theoretical value of the energy, should be parallel to each other. The calculations performed in this Letter should answer this question and give some esti-

Table 1

The calculated energy differences between particular conformers defined in Scheme 1 (kcal/mol)

	$E_{\text{I}} - E_{\text{II}}$			$E_{\text{I}} - E_{\text{III}}$			$E_{\text{II}} - E_{\text{IV}}$			$E_{\text{III}} - E_{\text{IV}}$		
	A	B	C	A	B	C	A	B	C	A	B	C
0	−8.65	−9.06	−9.57	−8.52	−9.32	−8.92	1.04	0.83	1.29	0.91	1.10	0.63
1a	−8.99	−9.32	−9.82	−8.61	−9.33	−8.99	1.30	1.08	1.46	0.91	1.08	0.63
1b	−6.13	−6.82	−6.64	−9.08	−9.90	−9.38	1.24	0.98	1.45	4.19	4.06	4.20
2a	−6.47	−7.12	−6.92	−9.11	−9.88	−9.48	1.48	1.22	1.60	4.11	3.99	4.15
2b	−6.33	−7.03	−6.78	−9.23	−10.04	−9.58	1.35	1.10	1.51	4.25	4.11	4.33
3	−6.49	−7.14	−6.85	−9.24	−10.0	−9.56	1.54	1.29	1.62	4.29	4.15	4.32

A-B3LYP/6-31G**, B-MP2/6-31G**, C-B3LYP/d95**.

Table 2

The calculated values of thermodynamic interactions (ΔH^0) and steric corrections: S_1 , S_2 , in kcal/mol

	ΔH^0			S_1			S_2			S'_2		
	A	B	C	A	B	C	A	B	C	A	B	C
0	-7.61	-8.22	-8.28	1.04	0.83	1.29	0.91	1.10	0.63	0.91	1.10	0.63
1a	-7.69	-8.24	-8.35	1.30	1.08	1.46	0.91	1.08	0.63	0.91	1.09	0.63
1b	-4.89	-5.84	-5.19	1.24	0.98	1.45	0.91	1.09	0.63	1.08	1.25	0.79
2a	-4.98	-5.93	-5.26	1.35	1.10	1.51	0.91	1.09	0.63	1.22	0.77	1.22
2b	-5.00	-5.89	-5.32	1.48	1.22	1.6	0.91	1.09	0.63	1.23	0.82	1.23
3	-4.95	-5.85	-5.24	1.54	1.29	1.62	0.91	1.09	0.63	1.22	0.74	1.22

A-B3LYP/6-31G**, B-MP2/6-31G**, C-B3LYP/d95**.

mation of the numerical values of particular contributions to the energy of intramolecular hydrogen bonding.

As the first step we apply the thermodynamic values of ΔH^0 , as they are directly calculated as a difference between states I and IV in order to estimate the additional elements of interactions S_1 and S_2 in compounds **0** and **1a**. Results are presented in Table 2.

As follows from Scheme 1, S_1 values can be directly taken from calculation as the energy differences between states II–IV (also given in Table 1).

The thermodynamic energy of the intramolecular O–H...N hydrogen bond in these two compounds is about -8 kcal/mol. Within each method of calculations one observes a small increase in the absolute values of ΔH^0 (on average about 0.06 kcal/mol) in this series, as the effect of substitution of the p-chlorine atom in DMAP. For these two molecules, ΔH^0 is equal to $\Delta H(\text{O–H...N})$. Within a particular method of calculation, S_1 shows a systematic increase of its value upon the chlorine substitution in the whole series. One can also expect systematic enhancement of ΔH^0 due to the increase of the acidity of the phenols. Table 2 shows, however, remarkably smaller differences between the energies of states I and IV in the **1b**, **2a**, **2b**, **3** series than those for compounds **0** and **1a**. This results from an additional stabilization, $\Delta H(\text{O–H...Cl})$, due to formation of the alternative O–H...Cl hydrogen bond in IV. This consequently leads to serious changes of the differences between states I and II, as well as between III and IV (as can see in Table 1).

S_2 can be directly obtained only for compounds **0** and **1a**. One can mention that these values are

almost identical for these two compounds, so one can assume that S_2 is nearly the same also for other compounds. The average values for compounds **0** and **1** are in Table 2 as are those of S_2 for **1b**, **2a**, **2b**, **3**.

Then, according to Scheme 1, the $\Delta H(\text{O–H...Cl})$ values were calculated using data from Table 1 and results are presented in Table 3.

2.2. Calculations based on results for chlorophenols

An alternative way of $\Delta H(\text{O–H...Cl})$ evaluation is carried out by independent calculations of the energy of the open and closed forms of ortho-chlorophenols. Calculated in such way, the $\Delta H(\text{O–H...Cl})$ values are also given in Table 3. Applying the last values, one obtains an alternative estimation of S'_2 values, which are given in Table 2. They are on average 20% higher than S_2 for compounds **0** and **1a**. One can state that the values of S'_2 do not change very much in the whole series. The $\Delta H(\text{O–H...Cl})$ values obtained from the thermodynamic cycle are a little bit higher than those obtained by direct calculation for *o*-chlorophenols (Table 3). It seems natural that such interactions could be enhanced in Mannich bases in the presence of an additional $-\text{CH}_2-\text{N}(\text{CH}_3)_2$ group. So one can take the last numbers for a better estimation of $\Delta H(\text{O–H...Cl})$ in the compounds **1b**, **2a**, **2b** and **3**. This shows an about 0.15 kcal/mol average increase in comparison with the values calculated for chlorophenols.

To obtain values of the energy of intramolecular hydrogen bonding ($\Delta H(\text{O–H...N})$) one has to correct the energy differences between IV and I on the effect of the intramolecular interaction O–H...Cl.

Table 3

The calculated values of $\Delta H(\text{O-H}\cdots\text{Cl})$ and $\Delta H(\text{O-H}\cdots\text{N})$ (kcal/mol)

	$\Delta H(\text{O-H}\cdots\text{Cl})$						$\Delta H(\text{O-H}\cdots\text{N})$					
	From thermod. cycle			From chlorophenols			From thermod. cycle			From chlorophenols		
	A	B	C	A	B	C	A	B	C	A	B	C
1b	-3.28	-2.98	-3.57	-3.11	-2.81	-3.41	-8.17	-8.82	-8.76	-8.00	-8.65	-8.60
2a	-3.34	-3.02	-3.70	-3.20	-2.89	-3.56	-8.32	-8.95	-8.96	-8.19	-8.82	-8.82
2b	-3.20	-2.90	-3.52	-3.04	-2.76	-3.33	-8.20	-8.79	-8.84	-8.04	-8.65	-8.66
3	-3.38	-3.06	-3.69	-3.24	-2.93	-3.58	-8.33	-8.91	-8.93	-8.19	-8.78	-8.82

A-B3LYP/6-31G**, B-MP2/6-31G**, C-B3LYP/d95**.

$$\Delta H(\text{O-H}\cdots\text{N}) = \Delta H^0 + \Delta H(\text{O-H}\cdots\text{Cl}).$$

The results are presented in Table 3, calculated for both variants of $\Delta H(\text{O-H}\cdots\text{Cl})$ estimation. The presented results show small differences between the particular methods of quantum mechanical calculation and similar trends, so one can use the average values for further discussion.

2.3. Correlation of $\Delta H(\text{O-H}\cdots\text{N})$ with other parameters characterizing the strength of hydrogen bonding

Applying the thermodynamic cycle and data for some external compounds to calculate additional interactions such as, $\text{O-H}\cdots\text{Cl}$, steric effects S_1 and S_2 , we were able to obtain $\Delta H(\text{O-H}\cdots\text{N})$, a thermodynamic characteristic of the intramolecular hydrogen bonding. The calculated average values are presented in Table 4 together with the energy differences between states I and II, the commonly used as the energy of hydrogen bonding, as well between states I and IV (ΔH^0 in our nomenclature) for comparison. The last two

characteristics are not able to reproduce the increase of hydrogen bonded interactions due to the growing number of chlorine substituents.

In the group of $\Delta H(\text{O-H}\cdots\text{N})$ values, we have two sets of data; the first set includes data from the thermodynamic cycle, calculated exclusively on data for structures I, II, III and IV. The second set uses data from the calculations on other molecules in order to determine the $\text{O-H}\cdots\text{Cl}$ interactions by use of chlorophenols with the same pattern of Cl-substitution as in particular Mannich bases. In the first case we made an approximation assuming the same values of S_1 in all compounds; in the second, assuming the same energy of $\text{O-H}\cdots\text{Cl}$ interaction in related phenols and Mannich bases. One can mention not very large differences between these two approaches.

2.4. Theoretical values of the energy of intramolecular hydrogen bond – ΔE_T

In the previous parts of Section 2 we considered the corrections on interactions in reference states used to calculate the hydrogen bond energy, such as $\Delta H(\text{O-H}\cdots\text{Cl})$. As was mentioned in Section 1 one can distribute the energy of the formation of intramolecular hydrogen bond into three components:

1. $\Delta H(\text{O-H}\cdots\text{N})$ – acid–base interaction between active groups.
2. Enhancement of steric interaction of the hydroxy group with other atoms of the chelate ring upon (S_2) formation of this ring.
3. Enhancement of steric interactions between the dimethyloaminomethyl group and the rest of the atoms of the chelate ring upon intramolecular hydrogen bond formation (S_1).

Table 4

Comparison of three different measures of intramolecular hydrogen bond energy (kcal/mol)

	$E_I - E_{II}$	ΔH^0	$\Delta H(\text{O-H}\cdots\text{N})$	
			From thermod. cycle	From chlorophenols
0	-9.09	-8.04	-8.04	-8.04
1a	-9.38	-8.10	-8.10	-8.10
1b	-6.53	-5.31	-8.58	-8.42
2a	-6.72	-5.39	-8.74	-8.61
2b	-6.84	-5.40	-8.61	-8.45
3	-6.83	-5.35	-8.72	-8.60

Because all the necessary components of the interactions have already been estimated in the previous parts, we can calculate ΔE_T

$$\Delta E_{\text{T}} = \Delta H(\text{O-H} \cdots \text{N}) - S_1 - S_2.$$

We have performed these estimations using, separately, the set of data with internal corrections (from the cycle) and with external ones (from calculations of model compounds such as chlorophenols). The results are given in Table 5. It can be mentioned that, independent of the method of portioning the energy of interactions, one obtains the same values of ΔE_T for particular compounds.

One can mention that the values of the energy of intramolecular interactions ΔE_T increase on 2–2.5 kcal/mol in comparison with $\Delta H(\text{O} \cdots \text{N})$. Steric interactions within the chelate ring diminish the commonly used estimations of intramolecular hydrogen bond energy. One can point out that best ΔE_T of all coincide with the values of differences between states III–I (Table 5). Using conformer III as a reference state, one avoids corrections on the large steric effect, S_1 , as well as on the energy of intramolecular $\text{O} \cdots \text{Cl}$ hydrogen bond. The ‘ideal’ reference state differs from III only by S_2 .

Fig. 1 present a pretty good correlation ($R^2 = 0.9937$) of the calculated values of ΔE_T with $r(\text{H} \cdots \text{N})$, which is a commonly used measure of the ability for the formation of hydrogen bonding and with $\rho(r)$ ($R^2 = 0.9909$) obtained from AIM [27] (Fig. 2). This confirms the reliability of the proposed approach.

3. Conclusions

Using three quantum mechanical methods, B3LYP/6-31G**, MP2/6-31G** and B3LYP/d95**, we have calculated the energy for five chloro-derivatives of 2-(*N*-dimethylaminomethyl)-phenols, in four different conformers each.

We have attempted to distribute the energy of intramolecular hydrogen bonding into three parts: acid–base interactions between the hydroxy group and the N atom, the steric interactions of the dimethylamino group with other atoms of the chelate ring, and the steric interaction of the

Table 5
The estimated parameters of the energy of intramolecular interactions in Mannich bases (kcal/mol)

	From thermodynamic cycle				From external data				
	$\Delta H(\text{O}-\text{H}\dots\text{N})$	S_1	S_2	ΔE_{T}	$\Delta H(\text{O}-\text{H}\dots\text{N})$	S_1	S_2	ΔE_{T}	III - I
0	-8.04	1.06	0.88	-9.98	-8.04	1.06	0.88	-9.98	-8.92
1a	-8.10	1.28	0.88	-10.25	-8.10	1.28	0.88	-10.25	-8.97
1b	-8.58	1.22	0.88	-10.68	-8.42	1.22	1.04	-10.68	-9.45
2a	-8.61	1.43	0.88	-10.92	-8.45	1.43	1.04	-10.92	-9.49
2b	-8.74	1.32	0.88	-10.94	-8.61	1.32	1.01	-10.94	-9.52
3	-8.72	1.48	0.88	-11.08	-8.82	1.48	1.00	-11.08	-9.60

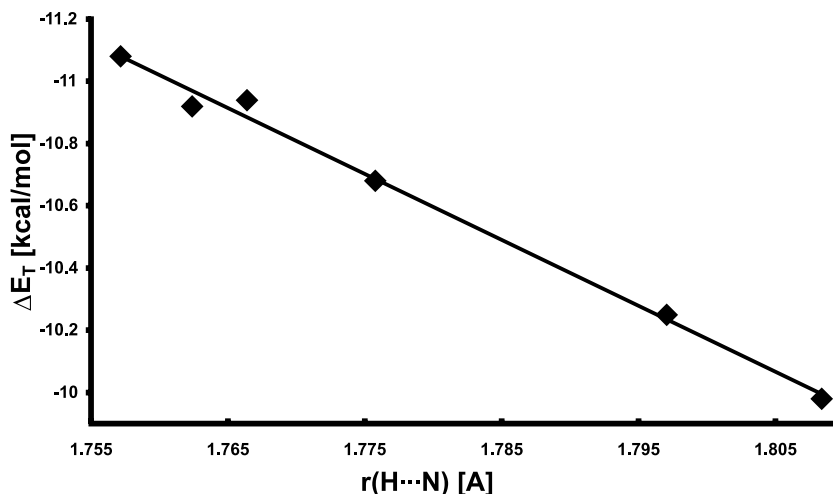


Fig. 1. Correlation between energy of hydrogen bond (ΔE_T [kcal/mol]) and $r(\text{H}\cdots\text{N})$ [Å] values.

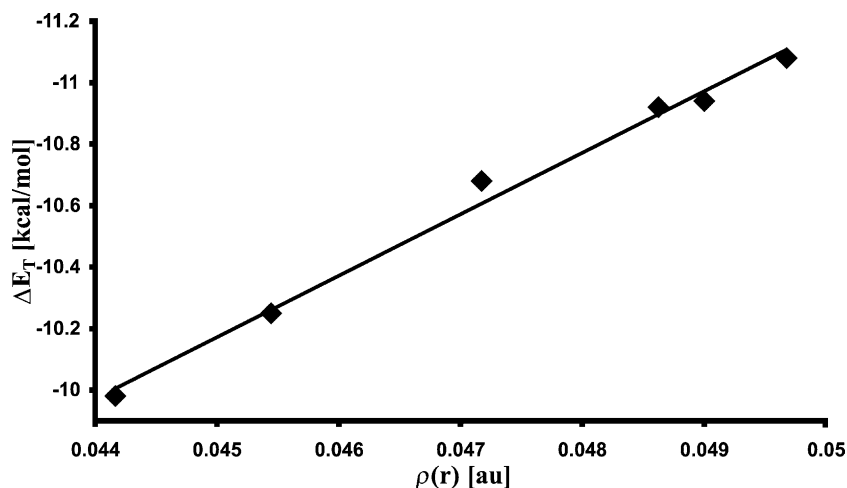


Fig. 2. Correlation between energy of hydrogen bond (ΔE_T [kcal/mol]) and electron density in the critical point of the hydrogen bond ($\rho(r)$ [a.u.]).

hydroxy group within the chelate ring. We have defined ΔH^0 , the thermodynamic energy of intramolecular hydrogen bonding, which is the energy difference between the hydrogen bonded form and the energetically lowest open form, $\Delta H(\text{O}-\text{H}\cdots\text{N})$, which describes the energy of the intramolecular hydrogen bond after corrections on $\text{O}-\text{H}\cdots\text{Cl}$ interactions in the open reference state, and finally ΔE_T , which includes the corrections for the steric interactions of the hydroxy and

N-dimethylaminomethyl groups in a closed chelate ring. Using the previously mentioned partition of the energy, we were able to estimate these three energetic components of intramolecular hydrogen bond. Taking into consideration the steric effects, one obtains an increase of estimated energy of the intramolecular hydrogen bond of 2–2.5 kcal/mol. Values of the ‘pure’ energy of the intramolecular hydrogen bond ΔE_T correlate well with $r(\text{H}\cdots\text{N})$ and electron density $\rho(r)$. The ΔE_T values can be

used directly to compare the energy of intra- and intermolecular hydrogen bonding.

Intramolecular interactions can be divided only to some extent into independent parameters, which are transferable between molecules. This is a reason why not all procedures of energy partition into components give equal results.

The obtained results are quite self-consistent in the group of six derivatives of *N*-(dimethylaminomethyl)-phenols studied in this work. Work on extension of the series of studied compounds is in progress.

From a practical point of view, to use a simplified definition of the energy of intramolecular hydrogen bond, one should select conformer III, not conformer II as a reference state.

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