

STUDY OF HYDROGEN BONDING IN CARBOXYLIC ACIDS BY THE MNDO/M METHOD

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Received July 2, 1993

Accepted October 29, 1993

The semiempirical methods MNDO/M, AM1 and PM3 were applied to the study of hydrogen bonds in carboxylic acids. The calculated hydrogen bond lengths and enthalpies of dimerization were compared with experimental data. The AM1 method fails to properly describe systems with strong hydrogen bonds. The PM3 method predicts the hydrogen bond lengths correctly but underestimates systematically the enthalpies of dimerization. MNDO/M appears to be a promising method for the treatment of association of carboxylic acids.

Carboxylic acids are among systems involving strong hydrogen bonds. In the gas phase, carboxylic acids form stable dimers up to their normal boiling temperature. As a consequence of the occurrence of hydrogen bonds, systems which involve carboxylic acids exhibit a strongly nonideal behaviour. Heterodimers are also present in carboxylic acid mixtures, rather scarce data relating to heteroassociation, however, are available. Experimental enthalpies of dimerization of carboxylic acids are given in Table I.

Theoretical investigation of the dimerization of carboxylic acids by using *ab initio* methods has largely concentrated on formic acid. The dimerization enthalpy values obtained by *ab initio* calculations differ from one another appreciably. While the value of enthalpy of association, $-63.2 \text{ kJ mol}^{-1}$, obtained for formic acid by del Bene and Kouchenour¹⁶ by calculation in the STO-3G basis set, agrees well with observed data, the data calculated by Smith¹⁷ and by Karpfen¹⁸ in the DZ basis set differ more than twofold (-49.4 and $-101.3 \text{ kJ mol}^{-1}$, respectively). The systematic treatment by Chang and coworkers¹⁹ demonstrates that the obtained enthalpy of dimerization depends strongly on the basis used. While calculation in the STO-3G basis set affords a value of $-52.7 \text{ kJ mol}^{-1}$ (this agreement, however, seems to be rather a fortuitous coincidence), the DZ basis set overestimates the enthalpy of dimerization, and only the DZ+P basis set gives satisfactory results again ($-51.5 \text{ kJ mol}^{-1}$). Similar results have been arrived at by Svensson and coworkers²⁰; calculation in the 6-31G+** basis set involving the diffusion functions ($-56.9 \text{ kJ mol}^{-1}$) was in a good agreement with the experiment. Inclusion of the correlation energy (at the MP2 level), however, again brings about

overestimation of the calculated dimerization energy ($-76.9 \text{ kJ mol}^{-1}$) because the stabilization energies are overestimated by MP2 method.

Formation of a cyclic dimer is associated with the appearance of six new vibrations and with a marked shift of the vibrational frequencies for the atoms involved. This fact has been confirmed by analysis of infrared spectra of formic¹⁹ and acetic²¹ acids. The *ab initio* calculated dimerization energy is therefore affected appreciably by changes in the zero point energy. According to Chang and coworkers¹⁹ the zero point energy contribution to the enthalpy of dimerization is about 10 kJ mol^{-1} , i.e. approximately 20% of the total value.

TABLE I
Experimental enthalpies of dimerization

Dimer (acids)	ΔH_{assoc} , kJ mol^{-1}	Method, ref.
Formic-formic	-59.06	P-V-T data ¹
	-61.92	spectra ²
	-58.99	spectra ³
	-48.90	spectra ⁴
Acetic-acetic	-69.92	P-V-T data ¹
	-68.20	spectra ⁵
	-60.30	spectra ⁶
	-61.09	spectra ²
	-59.40	spectra ³
Propionic-propionic	-63.48	P-V-T data ⁷
	-62.34	spectra ²
	-60.67	spectra ⁴
Butanoic-butanoic	-58.16	P-V-T data ⁸
	-65.69	spectra ²
2-Methylpropanoic-2-methylpropanoic	-63.60	spectra ²
Trimethylacetic-trimethylacetic	-61.10	spectra ²
	-58.58	P-V-T data ⁹
Heptanoic-heptanoic	-56.06	P-V-T data ⁸
Acrylic-acrylic	-77.39	P-V-T data ¹
Benzoic-benzoic	-68.00	spectra ¹⁰
Trifluoroacetic-trifluoroacetic	-58.44	P-V-T data ⁸
	-58.79	P-V-T data ¹¹
Chloroacetic-chloroacetic	-60.57	P-V-T data ¹²
Dichloroacetic-dichloroacetic	-60.70	P-V-T data ¹²
Formic-acetic	-61.12	P-V-T data ¹³
Formic-trifluoroacetic	-66.11	spectra ¹⁴
Acetic-trifluoroacetic	-69.46	P-V-T data ¹⁵

Study of hydrogen bonding in carboxylic acids by standard semiempirical method does not lead to good results. The AM1 method²² gives values about -25 kJ mol^{-1} for formic, acetic and acrylic acids²³, whereas the PM3 method^{24,25} affords ΔH_{assoc} values of approximately -35 kJ mol^{-1} for formic, acetic and benzoic acids²⁶. Several modifications of the MNDO method^{27,28} have therefore been proposed to calculate systems which involve hydrogen bonding, viz. the MNDO/I method²⁹ applied to water association and the MNDO/H (ref.³⁰) and MNDO/M (ref.³¹) methods which are modifications of the former. The two last-mentioned methods are based on a special approach to the calculation of the core-core repulsion for atoms making up the hydrogen bond. In the conventional MNDO method, this repulsion is calculated as

$$E_{\text{AB}} = -Z_{\text{A}}Z_{\text{B}}\gamma_{\text{AB}}[1 + f(R_{\text{AB}})]. \quad (1)$$

The empirical function $f(R_{\text{AB}})$ is expressed in the form of an exponential of the first power of the R_{AB} internuclear distance. In the MNDO/M method the function $f(R_{\text{AB}})$ of atoms involved in the hydrogen bond is expressed in the form

$$f(R_{\text{AB}}) = \sum_{i=1}^2 A_{\text{X}_i} e^{-C_{\text{X}}(R_{\text{HX}} - B_{\text{X}_i})^2}, \quad (2)$$

where R_{HX} is the internuclear distance of atoms X and H, and A_{X_i} , B_{X_i} and C_{X} constitute a set of additional five parameters.

The MNDO/H method has been applied to the calculation of the enthalpy of dimerization of formic and benzoic acids³². While the result for the former, viz. -44 kJ mol^{-1} , is fairly satisfactory, that for benzoic acid, -110 kJ mol^{-1} , is overestimated strongly in comparison with the experiment. The MNDO/M method has been used in the study of association of simple anions with water³¹ and of amino acids with water³³. In the former case the results were compared with nonempirical calculations in the 6-31G** base. The dimerization enthalpies obtained by the MNDO/M method were in a good agreement with *ab initio* calculations as well as with experimental data, whereas the molecular geometries found by the MNDO/M method and by *ab initio* calculations exhibited differences. No reliable experimental data for a comparison of the calculated results were available in the latter case. An assessment of the applicability of the MNDO/M method to the study of association of carboxylic acids is the subject of the present work.

CALCULATIONS

The systems given in Table I were studied by the MNDO/M method and, for a comparison, by the AM1 and PM3 methods. Computer program VAMP (ref.³⁴) was run on an IBM-PC 486. The most stable conformation, viz. the hydrocarbon chain and the C=O group in the *trans* position, was considered for all monomers and dimers. The calculations included complete molecular geometry optimization.

RESULTS AND DISCUSSION

Molecular Geometry

The hydrogen bond lengths, i.e. the O...H...O internuclear distances, in the carboxylic acid dimers as obtained by the three methods are given in Table II. The results calculated by the AM1 method for formic, acetic and acrylic acids agree well with those of ref.²³, those calculated by the PM3 method are consistent with those by Jurema and Shields²⁶.

TABLE II
Calculated O...H...O internuclear distances

Dimer (acids)	r_{OO} , nm		
	MNDO/M	AM1	PM3
Formic-formic	0.278	0.307	0.274
Acetic-acetic	0.277	0.306	0.273
Propionic-propionic	0.280	0.306	0.276
Butanoic-butanoic	0.280	0.306	0.276
2-Methylpropanoic-2-methylpropanoic	0.279	0.306	0.275
Trimethylacetic-trimethylacetic	0.279	0.307	0.274
Heptanoic-heptanoic	0.280	0.306	0.275
Acrylic-acrylic	0.280	0.306	0.275
Benzoic-benzoic	0.277	0.304	0.274
Trifluoroacetic-trifluoroacetic	0.281	0.309	0.276
Chloroacetic-chloroacetic	0.279	0.310	0.278
Dichloroacetic-dichloroacetic	0.279	0.306	0.277
Formic-acetic	0.280	0.307	0.278
Formic-trifluoroacetic	0.278	0.308	0.275
Acetic-trifluoroacetic	0.280	0.307	0.279

Experimental O...H...O distances are only available for several dimers. For homodimers the data have mostly been obtained by electron diffraction measurements. Karle and Brockway³⁵ report a value of 0.273 nm for formic acid, whereas a more recent value by Almenningen and coworkers³⁶ is 0.2703 nm. A value of 0.276 nm was found for acetic acid, ref.³⁵ gives 0.268 nm. A length of 0.2711 nm has been found experimentally for propionic acid³⁸. Costain and Sristava¹⁴ used microwave spectroscopy to study heterodimers which involved trifluoroacetic acid. The O...H...O distances are 0.269 nm in the formic acid–trifluoroacetic acid dimer and 0.267 nm in the acetic acid–trifluoroacetic acid dimer.

Table II demonstrates that the PM3 and MNDO/M methods produce O...H...O distances with a reasonable accuracy (the average errors are 0.005 and 0.007 nm, respectively), whereas the AM1 method overestimates the hydrogen bond lengths systematically (average error 0.037 nm). All of the methods predict linear O...H...O bonds.

Proton Shifts

In carboxylic acid dimers, the hydrogen protons shift from the O–H bond towards the C=O bond. The displacement occurs via a transition state with an energy maximum. This phenomenon has been studied by *ab initio* calculations for formic acid^{20,39} and for benzoic acid³², where the equilibrium geometry possesses the C_{2h} symmetry whereas the transition state possesses the D_{2h} geometry.

The potential barrier V_0 in the proton displacement, defined as the energy difference between the transition and stable states, as well as the O...H distances corresponding to the energy maximum were calculated by the MNDO/M method. A simultaneous shift of both protons was considered in heterodimers. This follows from the calculated geometries, where the structure of the ring in $R_1-(COOH)_2-R_2$ dimers is little dependent on the nature of the substituents R_1 and R_2 (Table II). The lengths of the two O–H bonds in the heterodimers differ less than 0.0015 nm.

The results of calculations are given in Table III. The data indicate that the O...H internuclear distances in the transition states (denoted $r(O-H)_{max}$) and the V_0 barrier heights are not very different for the various dimers. The O...H internuclear distance is longer in the transition state than in the stable state. The V_0 value for benzoic acid is appreciably lower than the value of 116.5 kJ mol⁻¹ obtained by the MNDO/H method but is consistent with the value of 53.1 kJ mol⁻¹ obtained within the same study by *ab initio* calculation in the 4-31G basis set. The V_0 barrier values calculated in different basis sets are also mutually different. The MNDO/M value agrees best with the *ab initio* calculation in the 6-31G+** basis set, which is also in accordance with the experiment with respect to the dimerization enthalpy calculation²⁰ ($V_0 = 71.5$ kJ mol⁻¹, $\Delta H_{assoc} = -56.9$ kJ mol⁻¹).

Enthalpy of Dimerization

The calculated enthalpies of dimerization (per dimer, i.e. two hydrogen bonds) and their errors are given in Table IV, demonstrating that the AM1 and PM3 methods underestimate the enthalpies of dimerization markedly (average errors of 35.8 and 27.3 kJ mol⁻¹, respectively). The MNDO/M methods gives enthalpies of dimerization with an average error of 3 kJ mol⁻¹. The experimental values given in Table I differ by 3 – 6 kJ mol⁻¹ for the various acids. Thus, the prediction of the enthalpy of dimerization by the MNDO/M method can be regarded as successful. The enthalpies of association of heterodimers are predicted by the MNDO/M method with a good accuracy as well.

Acrylic acid is an exception, where the error of the MNDO/M method is multiply higher than for the remaining dimers. Table I demonstrates that this acid is an anomaly in comparison to the other acids studied (the enthalpy of dimerization is nearly 20 kJ mol⁻¹ higher). On the other hand, all of the methods used exhibit markedly higher errors in the calculation of the enthalpy of formation for acrylic acid than for the other acids. This is apparent in Table V where the errors of the calculated enthalpies of formation $\Delta H_{f,298}^0$ are given in comparison with the experimental data⁴⁰. The error of the calculated enthalpy of dimerization of acrylic acid is comparable to that in its calculated enthalpy of formation.

TABLE III

The O...H internuclear distances in the transition state and the energy differences V_0 between the transition and stable states as calculated by the MNDO/M method for carboxylic acid dimers

Dimer (acids)	$r_{(\text{O}-\text{H})_{\text{max}}}$, nm	V_0 , kJ mol ⁻¹
Formic–formic	0.127	67.5
Acetic–acetic	0.127	69.1
Propionic–propionic	0.127	60.6
Butanoic–butanoic	0.127	68.5
2-Methylpropanoic–2-methylpropanoic	0.126	71.0
Trimethylacetic–trimethylacetic	0.128	69.6
Heptanoic–heptanoic	0.126	61.5
Acrylic–acrylic	0.128	64.4
Benzoic–benzoic	0.127	58.5
Trifluoroacetic–trifluoroacetic	0.128	71.8
Chloroacetic–chloroacetic	0.125	73.9
Dichloroacetic–dichloroacetic	0.128	70.8
Formic–acetic	0.127	67.7
Formic–trifluoroacetic	0.127	68.3
Acetic–trifluoroacetic	0.129	68.6

TABLE IV

Calculated enthalpies of dimerization ΔH_{assoc} and differences $\Delta = (\Delta H_{\text{assoc}})_{\text{obs}} - (\Delta H_{\text{assoc}})_{\text{calc}}$ with respect to average experimental values (all in kJ mol^{-1})

Dimer (acids)	MNDO/M		AM1		PM3	
	ΔH_{assoc}	Δ	ΔH_{assoc}	Δ	ΔH_{assoc}	Δ
Formic–formic	-59.20	-0.99	-26.57	33.42	-34.96	25.03
Acetic–acetic	-59.79	3.19	-25.69	37.29	-36.75	26.23
Propionic–propionic	-57.78	4.38	-26.51	35.65	-35.71	26.45
Butanoic–butanoic	-58.20	3.72	-26.16	35.77	-35.29	24.64
2-Methylpropanoic–2-methylpropanoic	-59.37	4.23	-28.16	35.44	-38.96	24.64
Trimethylacetic–trimethylacetic	-59.38	-0.46	-25.73	34.41	-35.27	24.57
Heptanoic–heptanoic	-56.92	-0.86	-24.82	31.25	-35.17	20.89
Acrylic–acrylic	-57.39	20.00	-25.00	52.39	-35.64	41.75
Benzoic–benzoic	-65.36	2.64	-25.24	42.76	-29.90	38.10
Trifluoroacetic–trifluoroacetic	-55.57	3.04	-25.27	33.34	-30.70	27.91
Chloroacetic–chloroacetic	-59.58	0.99	-27.35	33.22	-34.59	25.98
Dichloroacetic–dichloroacetic	-60.70	-0.13	-28.50	32.07	-34.10	26.47
Formic–acetic	-59.55	1.57	-25.81	35.31	-35.88	25.24
Formic–trifluoroacetic	-59.78	6.36	-27.33	-38.78	-34.72	31.39
Acetic–trifluoroacetic	-60.73	9.23	-27.13	42.33	-36.94	32.52

TABLE V

Differences between experimental and calculated enthalpies of formation of monomeric acids $\Delta = (\Delta H_{\text{f}, 298}^0)_{\text{obs}} - (\Delta H_{\text{f}, 298}^0)_{\text{calc}}$, (kJ mol^{-1})

Acid	MNDO/M	AM1	PM3
Formic	-8.63	-28.73	-16.80
Acetic	9.76	-1.91	6.05
Propionic	11.48	-2.71	8.66
Butanoic	14.51	-9.32	8.08
Heptanoic	15.89	-34.65	0.72
Acrylic	65.25	62.89	68.62
Benzoic	19.03	10.23	17.34
Trifluoroacetic	25.05	16.06	10.37
Chloroacetic	-9.88	-8.92	10.77

Population Analysis

The calculated enthalpies of dimerization of the acids studied are not appreciably different. This also applies to the O...H...O internuclear distances and potential barriers V_0 . The hydrogen bond strength can be assumed to be little affected by the nature of the groups bonded to the dimer ring. This assumption was verified by Mulliken population analysis. The overlap population values obtained by the MNDO/M method for bonds involved in the ring (i.e. O...H, O-H, C-O and C=O) are given in Table VI. The differences between the overlap populations for the various dimers are low. The populations at the O-H bonds differ by 0.04% on average, the highest deviation of 0.8% being observed for trifluoroacetic acid. For the C-O and C=O bonds the average deviation is about 1%; the highest deviation for the C-O bond occurs with trifluoroacetic acid (2.9%), for the C=O bond, with acetic acid (2.9%). The overlap populations at the O...H bond differ by 3.2% on average, trifluoroacetic acid exhibiting the highest deviation (4.3%). In absolute terms, however, this deviation is actually at the same absolute level as the deviations for the remaining bonds because the overlap population at the O...H bond is substantially lower than at the other bonds. The charge displacement in hydrogen-bonded complexes is defined by the equation

$$\Delta q = \sum_i (q_{\text{assoc}} - q_{\text{isol}}) , \quad (3)$$

TABLE VI

Overlap populations at bonds involved in the dimer ring

Dimer (acids)	O...H	O-H	C-O	C=O
Formic-formic	0.034	0.742	0.965	1.451
Acetic-acetic	0.032	0.746	0.957	1.446
Propionic-propionic	0.031	0.754	0.957	1.445
Butanoic-butanoic	0.032	0.742	0.950	1.448
2-Methylpropanoic-2-methylpropanoic	0.033	0.741	0.956	1.443
Trimethylacetic-trimethylacetic	0.032	0.745	0.953	1.447
Heptanoic-heptanoic	0.031	0.747	0.957	1.445
Acrylic-acrylic	0.033	0.745	0.958	1.432
Benzoic-benzoic	0.032	0.746	0.962	1.449
Trifluoroacetic-trifluoroacetic	0.030	0.739	0.989	1.497
Chloroacetic-chloroacetic	0.032	0.744	0.959	1.466
Dichloroacetic-dichloroacetic	0.031	0.742	0.968	1.471
Formic-acetic	0.031	0.742	0.961	1.450
Formic-trifluoroacetic	0.032	0.738	0.977	1.472
Acetic-trifluoroacetic	0.032	0.737	0.978	1.477

where q_{assoc} and q_{isol} are charges at atoms of the associate and at the isolated molecule, respectively, and the summation is performed over all atoms of the molecule which is regarded as the donor or acceptor. In homodimers the Δq value is zero, and in the formic acid–acetic acid heterodimer it is negligible. In systems involving trifluoroacetic acid the charge is markedly shifted towards that acid, which acts as the acceptor. For the formic acid–trifluoroacetic acid and acetic acid–trifluoroacetic acid dimers the Δq value is 0.014, which is comparable to the values observed for systems involving water and alcohols^{26,35}.

Consistent with the results are the dipole moment values. In the homodimers the calculated dipole moments are lower than 0.1 D whereas in the formic acid–acetic acid heterodimer the dipole moment is 0.54 D. Values of 3.37 and 3.79 D were obtained by the MNDO/M method for the formic acid–trifluoroacetic acid and acetic acid–trifluoroacetic acid heterodimers.

CONCLUSIONS

The AM1 method is unsuitable for the treatment of systems involving strong hydrogen bonds: it gives neither reliable hydrogen bond lengths nor reliable enthalpies of dimerization. The PM3 method predicts the hydrogen bond lengths with a satisfactory accuracy and thus is applicable to the study of molecular geometries of associate-type complexes but it is unsuitable for the prediction of hydrogen bond energies. The MNDO/M method gives good results in the description of both the geometrical and energy parameters of the hydrogen bonds. Since the parameters of this method have been evaluated from properties of systems involving hydrogen bonds weaker than in carboxylic acids (water-containing complexes), the method can be expected to be well applicable to the study of hydrogen bonds of diverse kinds.

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Translated by P. Adamek.