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The Hydrogen Bonding in Solids. Part I. The Hydrogen Bonding Model for the O—H...O Systems in Crystals of Carboxylic Acids

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New potential functions are presented for the the O—H···O systems. Various correlations are shown for carboxylic acids in the crystal. The H-bond energy calculated from the new model corresponds to that obtained from the Lippincott and Schroeder model and to the difference between the unity and the sum of the Pauling bond number.

INTRODUCTION

To understand the small distortions in the geometry of molecules in crystals it is necessary to study intermolecular forces. Among them, hydrogen bonding is a very strong intermolecular interaction.

Many theoretical approaches to explaining the H-bond have been proposed. A number of monographs and extended reviews in this field have been published. We can mention those which appeared after 1970, *i. e.*, review articles concentrating on the *ab initio* calculations.[1–4] The most interesting for our purposes are those describing O—H . . . O systems in the crystalline state, statistical and quantum-chemical analysis,[5] description of the isotope effect and its application to symmetric bonds,[6] H-bond geometries determined by neutron diffraction.[7]

Among several empirical or semi-empirical models of the hydrogen bond which have been suggested and which allow one to calculate H-bond energy, that developed by Lippincott and Schroeder[8] has enjoyed reasonable success and has been applied to many cases. As one example we can consider the case of the hydrogen bond model introduced by Derissen and Smit[9] for carboxylic acids.

Carboxylic acids are often intensively studied in terms of intermolecular interactions.[10] The *ab initio* calculations have been also done for the simple system of formic acid dimer[11–13] and for more complex systems. As an example we can mention the calculations for the benzoic acid dimer.[14] Therefore, the existence of the H-bond model for carboxylic acids is very convenient.

Carboxylic acids have also been investigated systematically by Ichikawa,[15] particularly the changes in the geometry of carboxylic group in the solid state.

These changes are often due to a disorder phenomenon in the solid state.[10,16]

The aim of this paper is to construct the hydrogen bonding model convenient for systems in the crystalline state and to analyze the influence of the crystal lattice over the geometry and the stabilization of H-bridge.

Carboxylic acids are useful for testing this model.

THE MODEL OF HYDROGEN BONDING

The best known model of hydrogen bonding is that of Lippincott and Schroeder.[8] The potential energy for this model consists of the sum of four terms:

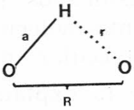
$$V = V_1 + V_2 + V_3 + V_4. \tag{1}$$

For example, for the system O—H . . . O, V_1 is the potential energy of the O—H bond, V_2 is the energy of the H . . . O bond and V_3, V_4 are terms of interaction between the oxygen atoms, V_3 — repulsion, V_4 — electrostatic term.

In this paper we propose for the O—H . . . O systems the potential energy consisting of the sum of three terms:

$$V = A/R^{12} - B/R^2 + C/r^{12} - D/r^6 + E/a^{12} - F/a^6 \tag{2}$$

i. e. the interactions between the pairs of atoms in H-bridge:



The O—H and H . . . O terms are of the Lennard-Jones type. The O . . . O interaction is composed of the repulsion term of A/R^{12} type and the attraction of $-B/R^2$ type.

It is well known that the following conditions characteristic of a stable equilibrium are applicable:

$$\left(\frac{\partial V}{\partial R}\right)_{\mathrm{eq}(R = R_o)} = 0; \quad \left(\frac{\partial V}{\partial r}\right)_{\mathrm{eq}(r = r_o)} = 0; \quad \left(\frac{\partial V}{\partial a}\right)_{\mathrm{eq}(a = a_o)} = 0 \tag{3}$$

$$\left(\frac{\partial^2 V}{\partial R^2}\right)_{\mathrm{eq}(R = R_o)} = k^{0}_{\mathrm{O}\cdots\mathrm{O}}, \quad \left(\frac{\partial^2 V}{\partial r^2}\right)_{\mathrm{eq}(r = r_o)} = k^{0}_{\mathrm{H}\cdots\mathrm{O}}, \quad \left(\frac{\partial^2 V}{\partial a^2}\right)_{\mathrm{eq}(a = a_o)} = k_{\mathrm{OH}}{}^{\circ}. \tag{4}$$

By using (2), (3) and (4) one obtains:

$$A = \frac{k^{0}_{\mathrm{O}\cdots\mathrm{O}}\ R_o{}^{14}}{120}, \qquad B = \frac{k^{0}_{\mathrm{O}\cdots\mathrm{O}}\ R_o{}^{4}}{20},$$

$$C = \frac{k^{0}_{\mathrm{H}\cdots\mathrm{O}}\ r_o{}^{14}}{72}, \qquad D = \frac{k^{0}_{\mathrm{H}\cdots\mathrm{O}}\ r_o{}^{8}}{36}, \tag{5}$$

$$E = \frac{k_{\mathrm{OH}}{}^{\circ}\ a_o{}^{14}}{72}, \qquad F = \frac{k_{\mathrm{OH}}{}^{\circ}\ a_o{}^{8}}{36}.$$

So, it is possible to construct the potential function (2) if the equilibrium values of a_o, r_o, R_o and of the force constants are available.

If two molecules joined together by H-bridge form a dimer we can define the hydrogen bonding in the following way. The hydrogen bond energy is the difference between the energy of the dimer and the energy of two mers.

From (2) and (5) the following expression is obtained for the hydrogen bond energy:

$$V(R, R_o) = V_{\text{dim}} - 2\,V_{\text{mer}} = \frac{k^0_{\text{O}\cdots\text{O}}\,R_o^{14}}{120\;R^{12}} - \frac{k^0_{\text{O}\cdots\text{O}}\,R_o^{4}}{20\,R^{2}} + \frac{k^0_{\text{H}\cdots\text{O}}\,r_o^{14}}{72\,r^{12}} - \tag{6}$$

$$\frac{k^0_{\text{H}\cdots\text{O}}\,r_o^{8}}{36\,r^{6}} + \frac{k_{\text{OH}}^{\,o}\,a_o^{14}}{72\,a^{12}} - \frac{k_{\text{OH}}^{\,o}\,a_o^{8}}{36\,a^{6}} + \frac{k_{\text{OH}}^{\,o}\,a_o^{2}}{72}$$

The last term of expression (6) given with the opposite value is the minimal energy of the O—H bond unperturbed by crystal lattice. The O—H bond is perturbed not only by H...O interaction but also by lattice forces, the energy of O—H depends on its length a and is of the Lennard-Jones type:

$$f(a, a_o) = \frac{k_{\text{OH}}^{\,o}\,a_o^{14}}{72\,a^{12}} - \frac{k_{\text{OH}}^{\,o}\,a_o^{8}}{36\,a^{6}}\,. \tag{7}$$

Replacing R_o by R, r_o by r, and a_o by a we can obtain from eq. (6):

$$V(R) = -\frac{k_{\text{O}\ldots\text{O}}\,R^2}{24} - \frac{k_{\text{H}\ldots\text{O}}\,r^2}{72} \tag{8}$$

We assume that expression (8) is the energy of the H-bond equilibrium system for the given crystal structure.

If the equilibrium geometry of the H-bond in the gas phase is known, *i. e.* if $R = R_o$, $r = r_o$, $a = a_o$, one can write:

$$V(R_o) = -\frac{k^0_{\text{O}\cdots\text{O}}\,R_o^2}{24} - \frac{k^0_{\text{H}\cdots\text{O}}\,r_o^2}{72}. \tag{9}$$

We can assume that the geometry of the acetic acid dimer in the gas phase[17] is optimal with respect to energy.

According to the above assumption we can writte:

$$\begin{aligned} r_{\text{OH}}^{\,o} &= a_o = 1.03\ \text{Å}, \\ r^0_{\text{H}\cdots\text{O}} &= r_o = 1.654\ \text{Å}, \\ R^0_{\text{O}\cdots\text{O}} &= R_o = 2.684\ \text{Å}, \end{aligned} \tag{10}$$

where the constants are those of the acetic acid dimer.[17]

We also assume that:

$$k_{\text{OH}} = b_1 - c_1\,a$$

$$k_{\text{H}\ldots\text{O}} = b_2 - c_2\,r$$

$$k_{\mathrm{O}\ldots\mathrm{O}} = b_3 - c_3 R \tag{11}$$

in accordance with approximations given in previous papers.[18,19]

According to equations given below it is possible to assign the values of b_i and c_i ($i = 1, 2, 3$).

$$\begin{cases} \left(\dfrac{\partial V}{\partial a}\right)_{a=a_o} = 0 \\ b_1 - c_1 a_o = k_{\mathrm{OH}}{}^{o} \end{cases} \tag{12}$$

and in the same way for r and R bonds. Constant $k_{\mathrm{OH}}{}^{o}$, $k^{o}_{\mathrm{H}\cdots\mathrm{O}}$ and $k^{o}_{\mathrm{O}\cdots\mathrm{O}}$ are those of acetic acid[20] and correspond to the appropriate a_o, r_o and R_o bonds:

$$k_{\mathrm{OH}}{}^{o} = 5.3\ \mathrm{mdyne/Å};\quad k^{o}_{\mathrm{H}\ldots\mathrm{O}} = 0.27\ \mathrm{mdyne/Å}; \\ k^{o}_{\mathrm{O}\cdots\mathrm{O}} = 0.147\ \mathrm{mdyne/Å}. \tag{13}$$

After the calculation of coefficients b_i and c_i, one can obtain general expressions for force constants:

$$\begin{aligned} k_{\mathrm{OH}} &= 3\, k_{\mathrm{OH}}{}^{o} - \frac{2\, k_{\mathrm{OH}}{}^{o}}{a_o} a, \\ k_{\mathrm{H}\ldots\mathrm{O}} &= 3\, k^{o}_{\mathrm{H}\ldots\mathrm{O}} - \frac{2\, k^{o}_{\mathrm{H}\cdots\mathrm{O}}}{r_o} r, \\ k_{\mathrm{O}\ldots\mathrm{O}} &= 3\, k^{o}_{\mathrm{O}\cdots\mathrm{O}} - \frac{2\, k^{o}_{\mathrm{O}\cdots\mathrm{O}}}{R_o} R_{\mathrm{O}\ldots\mathrm{O}}. \end{aligned} \tag{14}$$

Equations (14) have been obtained assuming that variables describing the geometry of hydrogen bond, R, r, and a are independent. From eq. (9) one can calculate the hydrogen bond energy:

$$V(R_o) = -7.81\ \mathrm{kcal/mol}. \tag{15}$$

This is the least H-bond energy for the set of constants given here. The force constants have been obtained in mdyne/Å units; $V(R, R_o)$, $V(R)$ and $V(R_o)$ in mdyne · Å. Distances are given in Å units. So, the coefficient for obtaining V's in kcal/mol has been introduced. It is equal to 143.53 kcal/mol : mdyne · Å.

Finally, the constants A, B, C, D, E and F of eq. (2) have the values:

$$\begin{aligned} A &= 177024.73 \\ B &= 54.746968 \\ C &= 617.26411 \\ D &= 60.295929 \\ E &= 15.98112 \\ F &= 26.767872 \end{aligned} \tag{16}$$

These constants allow us to use R, r and a in Å units and to obtain V in kcal/mol.

RESULTS AND DISCUSSION

In the previous section we obtained the expressions for $V(R, R_o)$, $V(R)$ and $V(R_o)$. Their physical meanings have been explained. It is necessary to ascertain the following relation:

$$V(R, R_o) > V(R) > V(R_o). \tag{17}$$

Besides, we can define the following values:

$$E_{def} = V(R, R_o) - V(R_o) \tag{18}$$

as a deformation energy of H-bridge after transition from the gas phase to the solid state and

$$E_{stab} = V(R, R_o) - V(R) \tag{19}$$

as a maximum stabilization energy of H-bridge by the crystal lattice. It means that if unstable geometry of H-bridge is inserted in the crystal lattice, the intermolecular interactions usually defined as the packing forces try to stabilize that geometry. So, the H-bridge can have unsuitable energy $V(R, R_o)$, but if energy $V(R)$ is profitable and the difference $V(R, R_o) - V(R)$ is rather small the crystal lattice can stabilize this geometry of H-bond.

In other words, this geometry may be possible in the crystal under investigation but impossible in the gas phase.

To test our model of hydrogen bond we have considered a set of several structures of carboxylic acids. The geometries of H-bridges have been taken. We should treat this sample of structures as a random set because the X-ray H-positions are not accurate.

It is possible to present some relations. $V(R, R_o)$ *vs.* $R_{o\ldots o}$ (Figure 1) shows that there is no predominant term of the total energy. It is usually expected that the term describing the O . . . O interaction is the most important but in the case of our model there is no correlation $V(R, R_o)$ *vs.* $R_{o\ldots o}$.

Figure 2 and Table I show the correlation E_{LS} *vs.* $V(R, R_o)$. E_{LS} is the hydrogen bond energy calculated from the model of Lippincott and Schroeder[8] for carboxylic acids.

Figure 3 and Tables II, III show the dependence $- E_{stab}$ *vs.* $|1 - \Sigma n|$, where n is the bond number — a value introduced by Pauling[21], Σn is the sum of bond numbers of bonds O—H and H . . . O. It has been pointed out[22,23] that if the Σn for hydrogen bond is close to unity, the bond is energetically allowed.

Thus, one can expect that the correlation between E_{stab} and $|1 - \Sigma n|$ values holds, because we know that if E_{stab} is greater, the H-bridge is less stable and $|1 - \Sigma n|$ is greater.

Roughly speaking, we should have a correlation in our case. Figure 3 confirms this hypothesis.

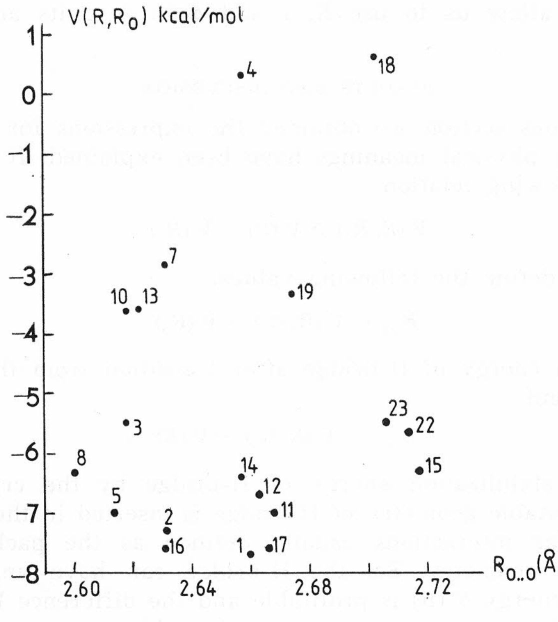


Figure 1. $V(R, R_o)$ *vs.* $R_{o\,..\,o}$.

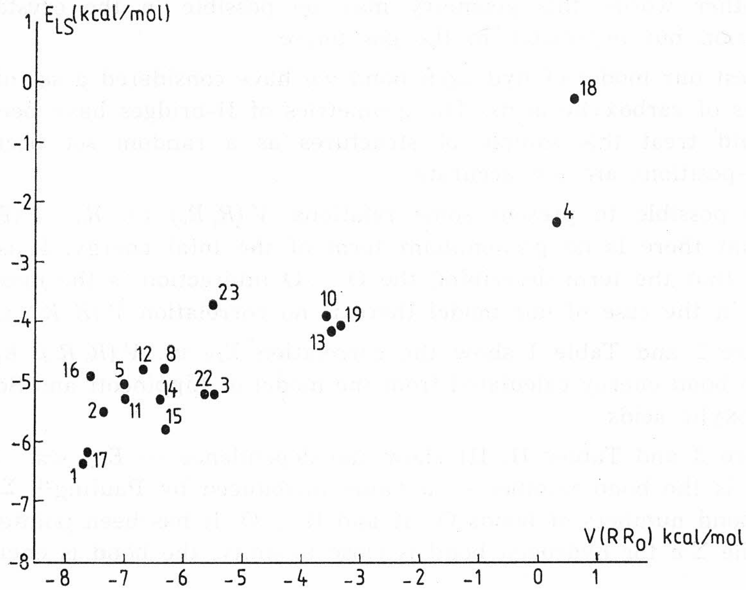


Figure 2. E_{LS} vs. $V(R, R_o)$.

Table III shows that in all cases the values of $V(R)$ are similar and that $V(R)$ tends to $V(R_o)$.

Thus, the value of (R, R_o) does not show a possibility of the existence of H-bond system in crystalline state. It means that in all cases the crystal

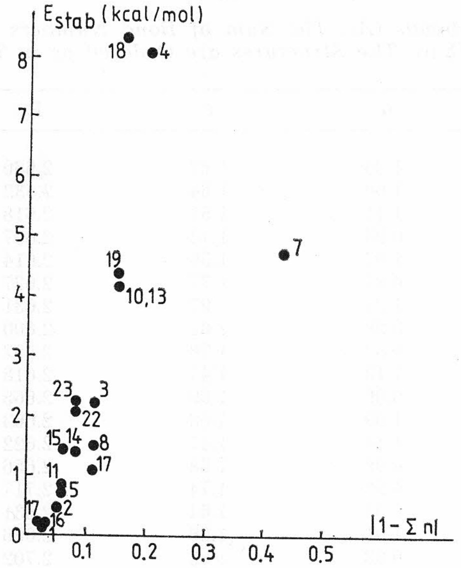


Figure 3. E_{stab} *vs.* $|1 - \Sigma n|$

TABLE I

The Values of H-bond Energy Calculated from the Lippincott-Schroeder Model^{+} *and from the Model Presented Here*$^{++}$ *(in kcal/mol); These Values have been Obtained for Benzoic Acid Derivatives*$^{1-15}$ *and for Linear Carboxylic Acids*$^{16-23}$

Acid	++	+	References
1. *p*-nitrobenzoic	—6.352	—7.738	24
2. *p*-metoxybenzoic	—5.470	—7.348	25
3. *p*-fluorobenzoic	—5.211	—5.503	26
4. *p*-hydroxybenzoic	—2.326	0.299	27
5. *p*-chlorobenzoic	—5.055	—7.017	28
6. benzoic	5.970	26.868	29
7. 2,3-dimetoxybenzoic	26.764	—2.849	30
8. *p*-*n*-butoxybenzoic (A)	—4.782	—6.333	31
9. *p*-*n*-butoxybenzoic (B)	3.581	20.062	31
10. *m*-metoxybenzoic	—3.874	—3.570	32
11. pentafluorobenzoic	—5.338	—6.974	33
12. mesitoic	—4.805	—6.724	33
13. 2,5-dinitrobenzoic	—4.151	—3.576	34
14. 2,4-dinitrobenzoic	—5.293	—6.428	35
15. 2,5-dihydroxybenzoic	—5.768	—6.337	36
16. acetic	—4.895	—7.613	37
17. trichloroacetic	—6.221	—7.608	38
18. α-oxalic	—0.250	0.635	39
19. β-oxalic	—4.062	—3.358	39
20. β-cyanoacetic	7.414	45.110	40
21. trifluoroacetic	1.942	9.823	41
22. hydroxyacetic (A)	—5.213	—5.648	42
23. hydroxyacetic (B)	—3.677	—5.524	42

TABLE II

The Geometries of H-bonds (Å); The Sum of Bond Numbers for Bonds O—H and H···O (Σ n). The Structures are Ordered as in Table I

	a	r	R	Σn
1.	1.04	1.62	2.660	0.97
2.	1.00	1.64	2.632	1.05
3.	1.11	1.51	2.618	0.89
4.	0.93	1.73	2.657	1.20
5.	1.07	1.56	2.614	0.94
6.	0.87	1.77	2.627	1.38
7.	1.21	1.97	2.631	0.57
8.	0.98	1.62	2.600	1.11
9.	0.88	1.78	2.652	1.34
10.	1.15	1.47	2.618	0.85
11.	0.99	1.69	2.668	1.06
12.	1.09	1.58	2.663	0.89
13.	1.15	1.47	2.622	0.85
14.	0.98	1.68	2.656	1.08
15.	0.98	1.74	2.717	1.06
16.	1.01	1.64	2.631	1.03
17.	1.01	1.66	2.666	1.02
18.	0.93	1.88	2.702	1.16
19.	0.95	1.73	2.674	1.15
20.	0.85	1.84	2.683	1.43
21.	0.90	1.78	2.648	1.27
22.	0.97	1.73	2.714	1.08
23.	0.97	1.77	2.696	1.08

lattice tries to stabilize the H-bridge to the minimum value of energy, *i. e.* to the energy of H-bond in the gas phase — $V(R_o)$. The important question is whether stabilization is possible or not, *i. e.* if E_{stab} is small or not.

Another conclusion directly arising from the above mentioned regularity $V(R) \rightarrow V(R_o)$ is the relation known from Table III:

$$E_{def} \approx E_{stab} \tag{20}$$

CONCLUSIONS

We present here a model of hydrogen bonding based on the assumption that three terms of interaction describe the energy of H-bridge, *i. e.* O . . . O, O—H and H . . . O. The model has been limited to the crystal structures of carboxylic acids. The limitation is induced by the choice of geometrical constants: R_o, r_o, a_o and force constants: k^{o}_{OH}, $k^{0}_{O\cdots O}$, and $k^{0}_{H\cdots O}$ taken from the data of the gasous acetic acid dimer. Constant c, useful for the calculation of the bond number, is also appropriate for crystal carboxylic acids. Another choice of constants may be useful for the other O—H . . . O systems.

From the results presented here one can see correlations E_{LS} *vs.* $V(R, R_o)$ and E_{stab} *vs.* $|1 - \Sigma n|$. It means that the new model is in agreement with the previous investigations.

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TABLE III

The Values of Energy:

a) $V(R)$ — +
b) $E_{def} = V(R, R_o) - V(R_o)$ — ++
c) $E_{stab} = V(R, R_o) - V(R)$ — +++

All Values are Given in kcal/mol and Ordered as in Table I

Acid	+	++	+++
1.	—7.802	0.072	0.065
2.	—7.798	0.462	0.451
3.	—7.763	2.302	2.255
4.	—7.794	8.109	8.093
5.	—7.779	0.793	0.762
6.	—7.774	34.678	34.642
7.	—7.616	4.962	4.768
8.	—7.785	1.477	1.452
9.	—7.776	27.872	27.838
10.	—7.744	4.240	4.174
11.	—7.803	0.836	0.828
12.	—7.796	1.086	1.072
13.	—7.745	4.234	4.169
14.	—7.802	1.382	1.374
15.	—7.790	1.473	1.454
16.	—7.798	0.197	0.185
17.	—7.805	0.202	0.197
18.	—7.715	8.445	8.350
19.	—7.796	4.452	4.438
20.	—7.745	52.920	52.855
21.	—7.775	17.633	17.598
22.	—7.787	2.162	2.139
23.	—7.781	2.286	2.256

REFERENCES

1. P. A. Kollman, *Modern Theoretical Chemistry, Applications of Electronic Structures Theory,* Ed., H. F. Schaefer, Plenum Press, **4** (1977) 109.
2. P. Schuster, *Intermolecular Interactions: from Diatomics to Biopolymers,* Ed., B. Pullman, J. Wiley, 1978.
3. K. Morokuma and K. Kitaura, *Molecular Interactions,* Ed., H. Ratajczak and W. J. Orville-Thomas, John Wiley and Sons Ltd., **1** (1980) 21.
4. A. Beyer, A. Karpfen, and P. Schuster, *Topics in Current Chemistry, Hydrogen Bonds,* Ed., P. Schuster, Springer-Verlag, Berlin, Heidelberg, New York, Tokyo, 1984.
5. J. Kroon, J. A. Kanters, J. G. C. M. Van Duijneveldt-Van de Rijdt, F. B. Van Duijneveldt, and J. A. Vliegenthart, *J. Mol. Struct.* **24** (1975) 109.
6. M. Ichikawa, *Acta Cryst.* **B34** (1978) 2074.
7. C. Ceccarelli, G. A. Jeffrey, and R. Taylor, *J. Mol. Struct.* **70** (1981) 255.
8. E. R. Lippincott and R. Schroeder, *J. Chem. Phys.* **23** (1955) 1099.
9. J. L. Derissen and P. H. Smit, *Acta Cryst.* **A34** (1978) 842.
10. L. Leiserowitz, *Acta Cryst.* **B32** (1976) 775.
11. H. Chojnacki, J. Lipiński, and A. Sokalski, *Int. J. Quantum Chem.* **19** (1981) 339.
12. S. Hayashi, J. Umemura, S. Kato, and K. Morokuma, *J. Phys. Chem.* **88** (1984) 1330.

13. S. J. Grabowski, T. M. Krygowski, G. Hafelinger, and G. Ritter, *Acta Cryst.*, submitted.
14. S. Nagaoka, T. Terao, F. Imashiro, A. Saika, N. Hirota, and S. Hayashi, *Chem. Phys. Lett.* **80** (1981) 580.
15. M. Ichikawa, *J. Cryst. Mol. Struct.* **9** (1979) 87.
16. S. J. Grabowski and T. N. Krygowski, *Mat. Sci.* **10** (1984) 85.
17. J. L. Derissen, *J. Mol. Struct.* **7** (1971) 67.
18. H. S. Johnston, *Adv. Chem. Phys.* **3** (1960) 131.
19. T. M. Krygowski and T. Więckowski, *Croat. Chem. Acta* **54** (1981) 193.
20. A. Novak, *Hydrogen Bonding in Solids,* in *Structure and Bonding* **18** (1974) 177.
21. L. Pauling, *J. Amer. Chem. Soc.* **69** (1947) 542.
22. H. B. Burgi, *Angew. Chem.* **14** (1975) 460.
23. S. J. Grabowski, *Croat. Chem. Acta* **61** (1988) 815.
24. M. Colapietro and A. Domenicano, *Acta Cryst.* **B33** (1977) 2240.
25. M. Colapietro and A. Domenicano, *Acta Cryst.* **B34** (1978) 3277.
26. M. Colapietro, A. Domenicano, and P. Ceccarini, *Acta Cryst.* **B35** (1979) 890.
27. M. Colapietro, A. Domenicano, and C. Marciante, *Acta Cryst.* **B35** (1979) 2177.
28. M. Colapietro and A. Domenicano, *Acta Cryst.* **B38** (1982) 1953.
29. R. Feld, M. S. Lehmann, K. W. Muir, and J. C. Speakman, *Z Kristallogr.* **157** (1981) 215.
30. R. F. Bryan and D. H. White, *Acta Cryst.* **B38** (1982) 1012.
31. R. F. Bryan and L. Fallon, *J. Chem. Soc. Perkin Trans.* **2** (1975) 1175.
32. G. W. Gridunowa *et al.*, *Kristallogr.* **27** (1982) 267.
33. V. Benghiat and L. Leiserowitz, *J. Chem. Soc. Perkin Trans.* **2** (1971) 1778.
34. S. J. Grabowski and T. M. Krygowski, *Acta Cryst.* **C41** (1985) 1224.
35. T. Więckowski and T. M. Krygowski, *Croat. Chem. Acta* **58** (1985) 5.
36. M. Haisa, S. Kashino, S.-I. Hanada, K. Tanaka, S. Okazaki, and M. Shibagaki, *Acta Cryst.* **B38** (1982) 1480.
37. P.-G. Jonsson, *Acta Cryst.* **B27** (1971) 893.
38. P.-G. Jonsson and W. Hamilton, *J. Chem. Phys.* **56** (1972) 4433.
39. J. L. Derissen and P. K. Smit, *Acta Cryst.* **B30** (1974) 2240.
40. J. A. Kanters, G. Roelofsen, and L. H. Straver, **B34** (1978) 1396.
41. I. Nahringbauer, J.-O. Lundgren, and E. K. Andersen, *Acta Cryst.* **B35** (1979) 508.
42. G. Roelofsen, J. K. Kanters, J. Kroon, H. M. Doesburg, and T. Koops, *Acta Cryst.* **B34** (1978) 2565.

SAŽETAK

Vodikova veza u krutinama. Dio I. Model vodikove veze za O—H···O sustave u kristalima karbonskih kiselina

S. J. Grabowski

Izvedene su nove potencijalne funkcije za sustave O—H···O. Prikazane su različite korelacije za karbonske kiseline u kristalu. Energija vodikove veze izračunana s pomoću novog modela odgovara onoj dobivenoj pomoću Lippincottova i Schroederova modela i onoj koja predstavlja razliku između jedinice i zbroja Paulingovih težina veza.