

the first to the second transition series or on altering the oxidation number of the metal atoms. Because changes of this sort can significantly change the strength and hence the bond distance, *without changing the bond order*, of multiple, especially quadruple, bonds, it is *not* permissible to employ arguments in which a simple, monotonic relationship between internuclear distance and bond order is posited. As we have said before,²⁰ but it still appears to need emphasis, "bond multiplicity is simply a measure of the number of electron-pair interactions and not a measure of bond strength (or length)".

It is interesting to note that since the completion of this work, Benard and Veillard²¹ have shown that the reason for the abject failure of the published LCAO-HF-SCF calculation¹² is, not too surprisingly, the failure of such a one-configuration calculation to take proper account of electron correlation. The usual method of taking some account of correlation within the framework of the HF-SCF approach is to introduce configuration interaction (CI), and Benard and Veillard have found that upon introducing a limited amount of CI (an expensive activity) a "completely different description of the bonding is achieved", namely, a Cr-Cr bond is found in the ground state.

In the one-configuration calculation,¹² the π -bonding (or what would have been) orbital lies at too high an energy to be occupied. Figure 2 shows one of the $6e_u$ orbitals which, according to our calculation, are the ones chiefly responsible for Cr-Cr π bonding; these orbitals *are occupied* in our picture, and as the contour diagram makes clear, they are of exactly the shape expected for an MO whose provenance, in an LCAO description, would be in pairs of overlapping $d\pi$ orbitals.

The ability of the SCF- $X\alpha$ -SW calculations reported here to give straightforwardly a correct ground-state picture of the $\text{Cr}_2(\text{O}_2\text{CH})_4$ molecule is noteworthy. It is attributed to the fact that, as Slater²² and others²³ have pointed out, the $X\alpha$ method automatically takes care of some parts of the correlation problem. It is for this reason, as is well-known, that SCF- $X\alpha$ -SW calculations generally give correct dissociation products for diatomics while (single-configuration) HF calculations frequently do not.²⁴

Finally, we note with satisfaction that within the limits of Koopman's theorem the patterns of calculated energy levels for $\text{Cr}_2(\text{O}_2\text{CH})_4$ in the Cr-Cr range 2.20–2.36 Å (which we are rather confident will include the actual values in the gaseous $\text{Cr}_2(\text{O}_2\text{CR})_4$ molecules) fit the reported¹² PES envelope very well. Thus, for the energies of the first few observed and first calculated ($2b_{2g}$) ionizations, calling the first one in each case zero, we have the following comparison, where we list observed energies followed by calculated ones in parentheses: 0 (0 for $2b_{2g}$), 0.45 (0.55 for $6e_u$), 1.55 (1.6 for $5a_{1g}$), etc. The reader may easily verify that there is semi-

quantitative agreement all the way to the $4e_u$ level of Figure 1 between the observed PES contour¹² and the calculated distribution of energy levels. We shall discuss the PES more fully when ionization energies have been calculated with allowance for relaxation.

Registry No. $\text{Cr}_2(\text{O}_2\text{CH})_4$, 63448-51-1.

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- (24) We are grateful to the National Science Foundation for partial support of this work.
- (25) Cf. the Bellman's dictum: "What I tell you three times is true." Lewis Carroll, *The Hunting of the Snark, Fit the First*, Verse 2.

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Hydrogen Halides and Hydrogen Bonds

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Sir:

A previous paper¹ on the strength of the hydrohalic acids put forth the following proposals: (a) hydrogen halide molecules in aqueous solution are hydrogen bonded to the water, and therefore the standard free energy of solution of HX(g) in water should be rather negative, and (b) the standard free energy of solution for all HX should be nearly constant and the same as for HF, namely, -5.6 kcal/mol.

Pauling² has taken issue with the assumption of hydrogen-bond formation and has also reiterated a previous proposal³ for estimating the ionization constants of the hydrogen halides. (His paper was overlooked in the literature search.) The present article is a more detailed examination of the available information of hydrogen bonding of hydrogen halides and its relevance to the question concerning hydrogen bonding to water.

Why a Hydrogen Bond? The intermolecular forces of attraction between molecules are generally ascribed mainly to dipole-dipole forces, dipole-induced dipole forces, and London or dispersion forces. For molecules which are free to

Table I. Covalent and van der Waals Radii, Å

Atom	van der Waals	Covalent	Atom	van der Waals	Covalent
N	1.5	0.70	Cl	1.8	0.99
O	1.4	0.66	H	1.2	0.30
F	1.35	0.64			

rotate the energy due to each of these is proportional to the inverse sixth power of the distance between the molecules. When one of the polar molecules involves hydrogen, then the distance of approach is significantly smaller. An idea of the effect of hydrogen can be obtained as follows.

Table I gives the covalent and van der Waals radii for a few small atoms. If we were to assume structures such as $-O\cdots O-O$ and $-O\cdots H-O$, where the solid line is a covalent bond and the dots represent van der Waals contacts, then the distances between centers of outer oxygen atoms will be respectively 5.12 and 3.2 Å. If these are raised to the sixth power, the results are 1.8×10^4 and 0.11×10^4 . It is plain that when hydrogen is involved in a polar molecule then the distance effect is very great and the energy of attraction is enough greater to warrant a separate name. (The hydrogen-bond distances are slightly shorter than ordinary van der Waals contacts.)

Hydrogen Bonding by Water. It is generally agreed that ice is held together by hydrogen bonds. Each water molecule is bonded by four hydrogen bonds, giving an average of two bonds per molecule. The calculations of the hydrogen bond energy can be made in various ways, depending somewhat on the definition of a hydrogen bond which is used.⁴

One can take the calculated enthalpy of vaporization of (hypothetical) ice at 298 K, 12.21 kcal/mol, and divide by 2 to get a hydrogen-bond strength of 6.1 kcal/mol of H bonds. (Unless otherwise specified the hydrogen-bond energies will be given as enthalpy changes, in kcal/mole of H bonds.) Or one can make a correction to 0 K, then eliminate the intramolecular and intermolecular zero-point energies, and obtain 6.7 kcal/mol.⁴ This is presumably the result which would be given by a rigorous quantum mechanical calculation.

There are some who wish to try to separate out the dispersion (and repulsion) forces and call the remainder the hydrogen-bond strength. Estimates have yielded values from 4.25 to 7.7.⁴ As suggested later, this separation is probably not justified, and the dispersion forces can make a significant contribution to the hydrogen-bond energy.

The hydrogen-bond energy in liquid water is probably very near the value in ice.⁵

The hydrogen-bond energy for the water dimer in the gaseous state has been measured to be 5.2 ± 1.5 kcal/mol.⁶ Perhaps one should not compare enthalpy changes for the rather different processes of $(H_2O)_2(g) \rightarrow 2H_2O(g)$ and $H_2O(s) \rightarrow H_2O(g)$. To make a more just comparison we should perhaps use the actual bond (internal) energy changes, $\Delta E_{\text{electronic}}$, with vibrations, rotations, and translations eliminated. For $(H_2O)_2(g) \rightarrow 2H_2O(g)$ this is 6.2 ± 1.5 kcal/mol.⁷ This is very close to the value of 6.7, previously quoted for ice. The hydrogen-bond energy in the vapor and solid are almost identical within experimental error.

Hydrogen Bonds Involving Hydrogen Halides. Direct measurements have not been made of hydrogen-bond strengths of HX with water. We must therefore proceed by comparison with other oxygen compounds, specifically the ethers, with similar polarity and electronic structure. Table II gives the results to date for reactions in the gaseous state. Fewer measurements have been made in solution; these are displayed in Table III.

The data clearly show that hydrogen bonds between HX and ethers (1) all have roughly the same energy with a trend of $HF > HCl > HBr$, (2) all are roughly equal to the hy-

Table II. Hydrogen-Bond Strengths (Enthalpies) for HX with Ethers, Gaseous State

Structure	Strength	Method	Ref
$Me_2O \cdots HF$	10.8	IR	9
$MeEtO \cdots HF$	8.8	IR	9
$Et_2O \cdots HF$	8.2	IR	9
$Me_2O \cdots HCl$	7.1	NMR	10
$Me_2O \cdots HCl$	7.0 ^a	Vp	11
$Me_2O \cdots HCl$	5.6, 6.9	IR	12
$Me_2O \cdots HCl$	7.1	IR	12
$Et_2O \cdots HCl$	7.5	IR	12
$Me_2O \cdots HCl$	6.7	Raman	13
$Me_2O \cdots HBr$	5.0	IR	12

^a Average.

Table III. Hydrogen-Bond Strengths (Enthalpies) for HX with Ethers, in Solution

Structure	Strength	Solvent	Method	Source
$Et_2O \cdots HCl$	6.4	Heptane	Vp	17
$Et_2O \cdots HCl$	7.4	Heptane	?	15
$Et_2O \cdots HCl$	6.1	Heptane	Vp	15
$(n-Pr)_2O \cdots HCl$	5.9	Heptane	Vp	17
$(n-Bu)_2O \cdots HCl$	6.0	$(n-Bu)_2O$	IR	14
$(n-Bu)_2O \cdots HCl$	5.9	CCl_4	IR	14
$(n-Bu)_2O \cdots HCl$	5.98	Heptane	?	15
$(n-Bu)_2O \cdots HCl$	6.1	Heptane	Vp	15
$(n-Bu)_2O \cdots HCl$	5.2	CCl_4	Vp	16
$(n-Bu)_2O \cdots HCl$	5.9	Heptane	Vp	17
$THF \cdots HCl$ ^a	6.5	Heptane	Vp	17
$THP \cdots HCl$ ^b	6.4	Heptane	Vp	17
$Et_2O \cdots HBr$	5.42	Heptane	Vp	15
$Et_2O \cdots HBr$	6.2	Heptane	?	15
$(n-Bu)_2O \cdots HBr$	5.37	Heptane (?)	?	15
$(n-Bu)_2O \cdots HBr$	5.42	Heptane	Vp	15

^a Tetrahydrofuran. ^b Tetrahydropyran.

drogen-bond energy of water, and (3) have very little solvent effect. Iogansen¹⁵ states: "on the basis of these results and other (qualitative) data, we suggest that the energies of hydrogen bonds of not too large molecules are relatively insensitive to the nearest environment of $A-H \cdots B$..." (This is not always true of course.)¹⁸ There are no comparable data for hydrogen iodide.

Thus the data, especially for HBr, negate the usual assertion:² "The electric dipole moments of the [larger] molecules are far less, and the ability to form hydrogen bonds is far less."

The Chemical Situation in Liquid Water. The current picture of liquid water^{19,20} is that the majority of the water molecules are still bonded in almost the same open-spaced manner as in ice, but some of the molecules have "fallen into" the holes and are relatively free. Probably a reasonable estimate of the number of "free" water molecules at room temperature is 5%. This corresponds to a concentration of 2.8 M. When these "free" molecules of H_2O react with HCl, there will be a decrease in entropy, of about $\Delta S = \Delta nR \ln 55.5$, where Δn is the decrease of moles in the reaction $H_2O + HCl \rightarrow H_2O \cdots HCl$. (The "free" water is treated as a solute.) The result is a $T\Delta S$ term of +2.38 kcal. If ΔH° is approximately -6 kcal/mol, then ΔG° is about -4 kcal. We will be quite conservative and reduce this to -2 kcal/mol and will also be conservative and reduce the "free" water to an assumed 1 M. The result is that 96% of the HCl is in the hydrogen-bonded form. The reaction of HCl with the 50 M hydrogen-bonded, high-structured water will have a ΔG° of about zero: it requires a bond breaking and bond forming with a net ΔH of about zero, and $T\Delta S$ will be near zero. We will again be conservative and assume ΔG° is about +1 kcal. If this assumption alone is true, then 90% of the HCl is in the hydrogen-bonded form. A further calculation shows that, if both

Table IV. Dipole Moments and Molar Polarizabilities of HX Molecules and Water

Molecule	Dipole moment, ^a D	Molar polarizability, cm ³
H ₂ O	1.85	3.9
HF	1.82	2.0
HCl	1.08	7.1
HBr	0.82	9.1
HI	0.44	13.5

^a R. D. Nelson, D. R. Lide, Jr., and A. A. Maryott, *Natl. Stand. Ref. Data Ser., Natl. Bur. Stand.*, No. 10 (1967).

conservative figures apply, then 97% of the HCl will be hydrogen bonded. Thus we conclude that virtually all HX molecules in aqueous solution are hydrogen bonded to the water by rather strong bonds of about 6 kcal/mol. (In low concentrations the HCl will not disturb the equilibrium between free and bound water molecules.)

Other Evidence Concerning Aqueous Solutions of HX. Bevan et al.²¹ have found evidence for the existence of the gaseous species H₂O...HF, but the microwave data provide no bond energy data.

Giglière²² found an absorption in the infrared spectrum which corresponds to the H₃O⁺ bending, modified to lower frequency, probably by a strong hydrogen bond to F⁻. This strongly bonded hydronium fluoride ion pair accounts for the low electrical conductivity of HF solution and other "deviant" properties. He felt that all of the thermodynamic data for HF will have to be recalculated to fit this new picture. If this is in fact true, then the great distinction between HF and other hydrogen halides disappears: HF is a strong acid just like the others. However, in this case it is virtually completely ionized but not completely dissociated. Giglière also found²³ a Raman absorption in supersaturated (i.e., under pressure) solutions of HCl and HBr which correspond to the HCl and HBr stretches, but shifted to lower frequency, probably by hydrogen bonding. There is now experimental evidence for the formation of hydrogen bonds by HX with water.

Summary and Interpretation. From the foregoing it can be seen that all the evidence, direct and indirect, points to HX molecules in aqueous solution which are hydrogen bonded to the water molecules with a strength virtually the same as that between water molecules. The strength of the bond appears to be about the same for all HX.

It seems strange at first glance that the larger halogens, with decreasing electronegativity, can form strong hydrogen bonds with such substances as ethers, ketones, and water. The explanation probably lies in the consideration of all the interactions involved in the attraction between molecules at short distances. These will be written out explicitly for the three chief contributions. (The first term applies only to freely rotating molecules, of course.)

$$\text{dipole-dipole attraction: } E_{\mu\mu} = \frac{-2\mu_1^2\mu_2^2}{3r^6kT} \quad (1)$$

$$\text{dipole-induced dipole attraction: } E_{\mu\alpha} = \frac{-2\alpha_1\mu_2^2}{r^6} \left(\frac{-2\alpha_2\mu_1^2}{r^6} \right) \quad (2)$$

$$\text{dispersion forces: } E_{\alpha\alpha} = \frac{-3\alpha_1\alpha_1(h\nu_0)}{4r^6} \quad (3)$$

Table IV gives some dipole moment and polarizability data relevant to this discussion.

The dipole moment of ethers or H₂O, μ_1 , is high and is the same in all the hydrogen-bonded species. The contribution of the dipole-dipole energy decreases as we proceed to larger halogens, and the dipole moment of HX decreases. However,

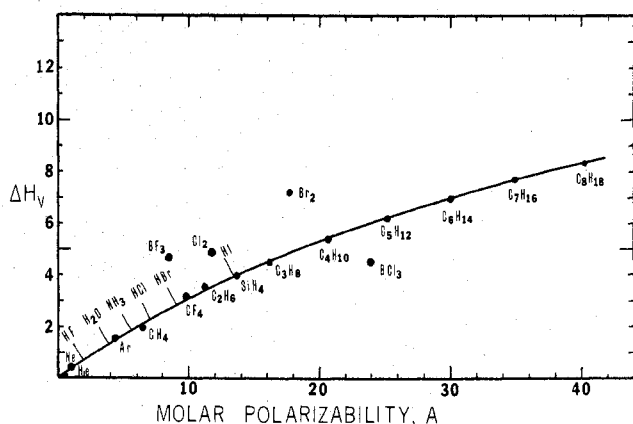


Figure 1. Molar heat of vaporization as a function of molar polarizability for nonpolar molecules.

the contribution of the second term in the dipole-induced dipole attraction remains quite large as we go down the series.

We can get some quantitative idea of the relative size of the dipole effects (first two equations) by substituting appropriate numbers in the equations. The dipole moments and (molar) polarizabilities are given in Table IV. For the structure H₂O...HX we will take the distance between centers to be as follows: van der Waals radius of O + van der Waals radius of H + covalent radius of H + covalent radius of X. Two sample results are

$$\text{HCl: } 71 \times 10^{-15} + (17 \times 10^{-15} + 106 \times 10^{-15}) = 188 \times 10^{-15} \text{ erg}$$

$$\text{HBr: } 33 \times 10^{-15} + (2.6 \times 10^{-15} + 91 \times 10^{-15}) = 131 \times 10^{-15} \text{ erg}$$

The ratio is 1.44. To these will be added the dispersion effect.

The contribution of dispersion forces can be a large part of the attraction between molecules. Figure 1 shows the molar heat of vaporization of several simple nonpolar compounds (at the normal boiling point) as a function of molar polarizability. (This enthalpy of vaporization will change a little when the temperature is changed.) From this curve we can estimate that the heats of vaporization of *nonpolar* H₂O, HF, HCl, HBr, and HI would be at least 1.3, 0.7, 2.2, 2.8, and 3.9 kcal/mol, respectively. This represents 10% of the actual heat of vaporization of HI but is 85% of the actual heat of vaporization of HF. Thus the dispersion contribution to the forces between molecules, and especially including H bonding, where the distances are somewhat shorter, cannot be neglected. The contribution to the bond energy will increase greatly in the series H₂O...HF, H₂O...HCl, and H₂O...HBr. When this amount is added to the dipole effects, the result is that the ratio of hydrogen-bond strengths for HCl and HBr is reduced to 1.2 (the experimental average ratio from Tables II and III).

Theoretical calculations have been made by Allen.²⁴ These calculations agree well with the limited experimental data for molecules with high dipole moments, but of low polarizability, such as (HF)₂ and (H₂O)₂, and for rather polarizable molecules, but with low dipole moments, such as (HCl)₂ and (H₂S)₂. There are no experimental data on the molecules of specific interest here, that is, molecules of high dipole moment and with high polarizability. However, we can make comparisons between calculations for H₂O with experimental data for ethers, the latter having almost the same geometry and electronic structure.

	Calcd	Ratio		Exptl	Ratio
F-H...OH ₂	11.4	2.0	F-H...OR ₂	9.5	1.4
Cl-H...OH ₂	5.7	1.5	Cl-H...OR ₂	6.9	1.2
Br-H...OH ₂	3.9		Br-H...OR ₂	5.8	

The calculated hydrogen-bond energy is given by

$$E_D = \frac{K\mu_{A-H}\Delta I}{R} \quad (4)$$

where μ_{A-H} is the dipole moment of the proton donor, ΔI a measure of the polarizability of the electron donor, R the internuclear separation, and K a constant. ΔI and K will be constant for the ethers. The dipole moments of HX are of course the same in the two sequences. The distance R will have the same relative values for H₂O and ethers. (If anything, the distance R will increase with larger HX, due to the interaction of X and the alkyl group. This would cause a sharper decrease in bond energies.) It can be seen that the relative values of hydrogen-bond energies should be the same for water and ethers. However, the data in the table show that the larger more polarizable HX compounds have higher values for bond energies. The hydrogen-bond energy is therefore not proportional to the dipole moment, as demanded by eq 4.

Registry No. H₂O, 7732-18-5; HF, 7664-39-3; HCl, 7647-01-0; HBr, 10035-10-6; HI, 10034-85-2.

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