Inorg. Chem. **1995**, *34*, 4004−4007

Electrostatic, Covalent, and Transfer Interpretation of Bond Strengths

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Received August 18, 1994

Introduction

In a recent series of articles,[1] the ECT model, eq 1, was reported to correlate and predict bond formation energies,

$$-\Delta H_{\mathrm{F}} = E_{\mathrm{ca}}E_{\mathrm{an}} + C_{\mathrm{ca}}C_{\mathrm{an}} + T_{\mathrm{ca}}R_{\mathrm{an}} \qquad (1)$$

$-\Delta H_{\mathrm{F}}$, *i.e.* minus the enthalpy of homolytic dissociation, ΔH_{D}. The parameters refer to atoms or radicals reacting to form a σ bond with the atom or radical forming the positive end of a polar bond referred to as the catimer (ca) and the atom or radical forming the negative end of a polar bond and animer (an). Following the bonding models of Kutzelnigg and Umeya and Morokuma,[3] $E_{\mathrm{ca}}E_{\mathrm{an}}$ refers to the electrostatic bonding contribution, $C_{\mathrm{ca}}C_{\mathrm{an}}$ the covalent contribution, and $T_{\mathrm{ca}}R_{\mathrm{an}}$ the electron transfer contribution. These contributions are arbitrarily broken up into catimer and animer components.

The set of parameters reported for the original bond energy fit[1a] subsequently were applied to an analysis of silicon[1c] and organometallic[1b] bond energies. In this report all of the data were combined to redetermine all the parameters. The addition of these and other[4] new systems helps to better define the minimum in the least-squares data fit leading to improved parameters. This article reports the new parameters.

The utilization of the parameters to analyze measurements other than enthalpies also is discussed and compared to other methods of analysis. Qualitative bonding models continue to be essential tools used frequently by experimental chemists in the design, interpretation, and extrapolation of the results from experiments. Extrapolations involve the prediction of properties of new compounds and lead to the selection of new compounds for a multitude of purposes. The more complete the bonding model, the better these predictions.

Results and Discussion

New Parameters. The new parameters from the combined fit of the data in ref 1 and additional data from ref 4 are reported in Table 1. These parameters can be used to calculate a bond energy by substituting the E_{ca}, C_{ca}, and T_{ca} values of the catimer into eq 1 along with the E_{an}, C_{an}, and R_{an} values of the animer. For homonuclear diatomics the catimer parameter for the atom must be combined with the animer parameter to determine the bond energy. For systems joined by a σ bond with no steric or π-bond stabilizing effects, the enthalpies are predicted to 1 kcal mol^{-1} or to within the experimental error of the measurement. When steric or π-bond stabilization exists, the deviation in the calculated and experimental value gives the magnitude of the effect.

The accuracy with which the parameters are known is indicated by their n-value. When $n \leq 2$ and ≥ 0.4, the parameters fit most of the enthalpies in the data fit to at least 1 kcal mol^{-1} and can be used to predict σ bond enthalpies on new systems to at least 1 kcal mol^{-1}. Parameters with $n \geq 0.4$ may not predict new systems accurately especially when the *C/E* or *C/T* ratios of the new system are outside the range employed in the data fit. In this case, the referenced literature can be consulted, and ΔH_{F} values for this new system can be added to all the previous systems to generate a series of simultaneous equations of the form of eq 1. Substituting known values of the animer (or catimer) leads to a series of equations that can be solved for refined values of the catimer (or animer). When the parameters for animers or catimers are used to analyze a new data set, the simultaneous equations are weighted as $1/n$.

As in ECW type analyses, accurate determination of parameters on new systems requires that the animers (or catimers) studied have different ratios of *C/E* or *C/T*. To define a catimer, substituents should include animers from at least four of the following groups: (I) alkyls and $-\mathrm{NH_2}$; (II) halogens and $\mathrm{OH^-}$; (III) $\mathrm{C_6H_5C{\equiv}C}$, $-\mathrm{CN}$; (IV) H, $\mathrm{C_6H_5}$, $\mathrm{CH_2{=}CH}$; (V) $-\mathrm{NO_2}$, $-\mathrm{SH}$, $-\mathrm{OCH_3}$, $-\mathrm{SCH_3}$. Those substituents in the above list with $n \geq 0.4$ are tentatively assigned to groups. To define a new animer, catimers should be selected from at least four of the following groups: (I) alkyls, $-\mathrm{C_6H_5}$; (II) H−, $J(^{13}\mathrm{C{-}H})$; (III) alkali metals and Zn; (IV) transition metals and the aluminum family; (V) halogen, catimers; (VI) organometallic catimers with T values ≥ 5 and *C/E* ratios ≥ 2.5.

Interpretations of the Parameters. Though devoid of quantitative determination or definition, the concepts of covalent and electrostatic bonding find widespread application by experimental chemists. Homonuclear diatomics are considered to be essentially covalent, and heteronuclear diatomics have varying degrees of covalency. Even the gas-phase $\mathrm{Na^+Cl^-}$ ion pair is acknowledged to have some covalency though there is no quantitative measure of the amount. In the ECT model, the trends in covalent character of bonds can be obtained from the ECTR parameters.

It is important to distinguish between the magnitude of the covalent contribution given by the $C_{\mathrm{ca}}C_{\mathrm{an}}$ product and the fraction covalent character in a bond given by eq 2. The

$$\text{fraction covalency} = \frac{C_{\mathrm{ca}}C_{\mathrm{an}}}{-\Delta H_{\mathrm{F}}} \qquad (2)$$

fractions are useful in discussing bond types while the trends in the *magnitude* of the covalent, electrostatic, and transfer contributions (*i.e.* the $E_{\mathrm{ca}}E_{\mathrm{an}}$, $C_{\mathrm{ca}}C_{\mathrm{an}}$, $T_{\mathrm{ca}}R_{\mathrm{an}}$ products) are best understood in terms of overlap and energy match consideration.

In the classification of molecules as ionic, polar covalent, or covalent, the fraction covalent character, $C_{\mathrm{ca}}C_{\mathrm{an}}/-\Delta H_{\mathrm{F}}$, is utilized. Values equal to or less than 0.2 are ionic, those greater than 0.2 are polar covalent, and homonuclear combinations are covalent. The homonuclear combinations generally have a fraction covalency greater than 0.7 except for $\mathrm{I_2}$. This exception does not arise because $\mathrm{I_2}$ is more ionic but because $\mathrm{I_2}$ has a large transfer energy contribution.

The transfer term is viewed as arising from the changes in the one center integrals on the individual atoms as the partial charge on the atom changes. The fact that the transfer term $T_{(\mathrm{ca})}$ does not plot up linearly with $E_{(\mathrm{ca})}$ or $C_{(\mathrm{ca})}$ or any linear combination thereof demonstrates the necessity of this separate

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(3) Umeyama, H.; Morokuma, K. *J. Am. Chem. Soc.* **1976**, *98*, 4400. Several contributions to bond strength are grouped into three categories by these authors. Though the trends are reproduced for the amines, questions about how to combine the contributions to produce a view of covalency for all donors that is consistent with qualitative trends remain.

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Table 1. Catimer and Animer Parameters for Use in Eq 1

Catimer Parameters[a]

catimer (n)	E_{ca}	C_{ca}	T_{ca}	catimer (n)	E_{ca}	C_{ca}	T_{ca}
$H-$ (0.2)	7.84	13.00	0.52	$Br-$ (0.5)	0.78	12.25	1.31
H_3C- (0.2)	4.00	11.83	3.37	$I-$ (0.2)	0.95	8.94	3.37
CH_3CH_2- (0.2)	4.27	11.45	3.41	$Mn-$ (0.4)	7.68	1.07	7.24
$(CH_3)_2CH$ (0.2)	5.06	11.04	2.37	$Co-$ (0.6)	8.37	2.88	5.31
$(CH_3)_3C-$ (0.2)	4.78	10.77	3.16	$Ni-$ (0.6)	7.44	4.51	6.57
H_5C_6- (0.6)	5.77	12.92	2.22	$Sc-$ (0.6)	12.34	1.28	5.27
$C_6H_5CH_2-$ (0.2)	2.36	10.22	4.59	$Cr-$ (0.6)	8.55	2.05	5.31
$CH_3C(O)-$ (0.6)	4.41	9.80	2.63	$Zn-$ (0.6)	5.53	0.01	4.03
H_3Si- (0.6)	9.13	10.12	1.22	$Cu-$ (0.2)	7.40	5.12	5.18
$(CH_3)_3Si-$ (0.6)	10.28	9.89	1.00	$Ag-$ (0.4)	6.30	4.11	5.63
$Li-$ (0.2)	10.98	2.77	6.43	η^5-Cp*IrP$(CH_3)_3H-$ (0.2)	3.77	6.42	9.96
$Na-$ (0.2)	8.03	1.48	7.47	η^5-CpRu$[P(CH_3)_3]_2-$ (0.2)	2.92	3.28	4.62
$K-$ (0.6)	9.99	0.26	8.00	DPPEPt$-$ (0.2)	2.90	1.02	5.45
$Rb-$ (0.5)	9.88	0.31	7.74	$(CO)_5Mn-$ (0.4)	2.83	4.71	8.82
$Cs-$ (0.5)	10.65	0.17	7.74	η^5-CpMo$(CO)_3-$ (0.4)	0.55	5.31	12.83
$Al-$ (0.4)	11.78	4.50	5.59	η^5-Cp_2Zr- (0.6)	7.63	7.06	8.74
$In-$ (0.5)	9.42	3.13	6.81	η^5-Cp'_3U- (0.4)	7.02	3.67	5.54
$Tl-$ (0.5)	8.07	1.81	6.69	η^5-Cp*ThOC$(CH_3)_3$ (0.4)	0.31	11.48	6.72
$Bi-$ (0.6)	4.12	7.33	4.60	$166 - J_{H_3{}^{13}C-}$[b] (0.3)	−1.17	6.50	0.89
$Cl-$ (0.6)	0.99	14.30	0.73	14 eV − IE[d] (1)	0	0	1.25

Animer Parameters[a]

animer (n)	E_{an}	C_{an}	R_{an}	animer (n)	E_{an}	C_{an}	R_{an}
$-H$ (0.2)	2.10	6.62	2.36	$-OCH_3$ (0.2)	5.07	4.97	1.14
$-CH_3$ (0.2)	2.36	6.66	0.60	$-NH_2$ (0.4)	3.98	5.78	0.53
$-CH_2CH_3$ (0.2)	1.77	6.70	0.20	$-NO_2$ (0.4)	4.13	3.47	1.28
$-CH_2CH_2CH_2CH_3$ (0.6)	1.56	6.51	0.36	$-SH$ (0.2)	3.44	4.78	1.11
$-H_2CC_6H_5$ (0.4)	0.89	6.12	0.18	$-SCH_3$ (0.4)	3.64	4.84	1.08
$-H_2CSi(CH_3)_3$ (0.6)	1.59	6.64	0.83	$-F$ (0.2)	9.81	4.45	2.52
$-H_2CC(O)CH_3$ (0.6)	2.12	6.23	1.24	$-Cl$ (0.2)	7.24	3.41	3.86
$-(O)CCH_3$ (0.4)	0.64	6.17	1.58	$-Br$ (0.2)	6.12	2.91	3.53
$-C_6H_5$ (0.2)	3.43	6.54	2.63	$-I$ (0.2)	5.14	2.23	3.26
$-CH{=}CH_2$ (0.2)	2.71	6.42	1.96	$-Au$ (0.2)	4.90	2.50	1.13
$-C{\equiv}CC_6H_5$ (0.4)	6.43	5.90	5.44	$-Ag$ (0.2)	1.39	3.12	2.53
$-CN$ (0.2)	5.52	6.19	5.87	$-Cu$ (0.2)	2.29	2.63	2.33
$-CF_3$ (0.6)	4.18	5.44	5.88	$-Bi$ (0.4)	1.45	5.05	1.07
$-CCl_3$ (0.6)	3.53	5.06	4.45	$\Delta e^2Qq(Cl)$[c] (0.4)	5.51	−0.42	7.18
$-OH$ (0.2)	7.12	4.76	2.55	E_A (1)	0	0	0.94
$-OC_6H_5$ (0.6)	3.86	4.04	0.77				

[a] An asterisk indicates a tentative parameter resulting from limited data. [b] The $^{13}C-H$ coupling constant for H_3C-X derivatives. The quantity calculated is $166 - J_{^{13}CH_3}$. The value of 166 is for an sp^2 carbon so the larger the number the closer to sp^3 the carbon hybridization. [c] The chlorine qudruple coupling constant for M−Cl compounds where chlorine is the animer. The e^2Qq(Cl) value + 109.7 is fit where 109.7 is the value for a free chlorine atom. [d] 14 electronvolts minus the ionization energy.

term for the quantitative fit of bond energies. The T_{ca} values do not plot up linearly with ionization energy nor does R_A with electron affinity. The transfer energies are treated by a product term which includes the diserpsion forces. The ionization energy and electron affinity are isolated atom properties that differ from transference and receptance which are molecular properties. Thus, the transfer term contributes to the polarity of the molecule but has other effects in it besides polarity as seen by the magnitude of the RT term for forming the nonpolar molecule, I_2, from atoms.

The transfer term has an important impact on the qualitative as well as the quantitative discussion of trends in bond strengths and chemical periodicity. The following generalizations, which refer to reactions of atoms or radicals, summarize the qualitative ideas used to incorporate the transfer components into the ionic and covalent bonding model: (1) The magnitude of the covalent contribution decreases as the size of the atoms in a family of elements increases. (2) The Coulomb interaction in a family decreases as the size of the catimer or animer increases. (3) The transfer contribution of the atom increases with decreasing ionization energies for monatomic systems, and the receptance of the atom increases with increasing electron affinity for monatomic systems. (4) When the groups attached to a bonding atom in a radical are varied, electron-releasing groups increase T and decrease R_{an}. Electron-attracting groups have the opposite effect.

In summary, when atoms combine to form a bond, transfer, ionicity, and covalent bonding determine the bond energy and the extent of electron transfer. When the energies of the AO's of the bonding electrons and HOMO's of the radicals are nearly the same for the catimer and animer (as crudely manifested by ionization energies), covalency makes the dominant contribution to the bonding. As the orbital energies differ, a polar bond is formed with significant contributions from ionic and transfer energies. As covalency decreases, the transfer term increases for monatomic catimers. Large monatomic catimers (low ionization energies) have larger transference than small monatomic catimers. Small, charged catimers have large electrostatic contributions because of the e^2/r_{ij} dependence of the energy. Large catimers undergo a weaker Coulomb interaction but have larger transfer energy contributions. These two opposite atomic properties (size and ionization energy) are the reason two independent terms are needed to account for the noncovalent contributions to the bonding and are the reason a two-term covalent−ionic description of the bond energies does not work. The new parameters have not changed[5] the trends in the parameters or any of the interpretations of the data fits reported earlier.

Thus, the ECT view of bonding provides a very different qualitative picture than that of electronegativity and requires a consideration of not only trends in ionicity and covalency but also transference to describe the chemical bond in the molecule. For qualitative predictions of trends, covalency is estimated by energy match and orbital overlap, ionicity by charge−size ratios, transference by the ionization energies of the catimer, and receptance by the electron affinities of the animer. The electronegativity scale has been of great utility for its intended use, the qualitative prediction of the direction of bond polarity in molecules. The E parameters for the animers can perform a similar function. The tendency of an animer to undergo electrostatic bonding includes those properties that tend to make it attract electron density and increase its partial negative charge in a molecule.

ECT Parameters as a Scale To Interpret Reactivity. The ECT parameters are the basis of a scale that enables one to determine if a physicochemical property is being determined by the same factors that influence bond energies. For example, some measured property, $\Delta\chi$, for a series of M−F compounds would be analyzed by substituting the E_{ca}, C_{ca}, and T_{ca} values for the various catimers, M, that were measured into the equation

$$\Delta\chi = E_{ca}E_{an}^* + C_{ca}C_{an}^* + T_{ca}T_{an}^* \qquad (3)$$

where an refers to fluorine. One equation results for each $\Delta\chi$, *i.e.*, each different M, and the series is solved for E_{an}^*, C_{an}^*, and R_{an}^*. The asterisk indicates that the fluorine animer parameter is for a physicochemical measurement other than the bond energy. A good fit of the data suggests the property is determined by the same factors that influence bond strength. A satisfactory fit is one in which the average absolute deviation in the measured and calculated values, $\bar{x}$, is comparable to the experimental error or is at most 6% of the range (high minus low) of the property measured. The deviation divided by the range expressed as a percentage is referred to as the percent fit. The electrostatic, covalent, and transfer components of the property are given by $E_{ca}E_{an}^*$, $C_{ca}C_{an}^*$, and $T_{ca}R_{an}^*$, respectively. When the catimer is held constant and the animer varied, the asterisk is placed on the catimer parameters and these are determined using known animer parameters.

The $J_{^{13}C-H}$ coupling constants[7] represent a spectral measurement that has been interpreted[1] with ECT. In the revised fit, the number of animers is expanded from 10 to 40. Twenty-one of the systems fit to better than 2 Hz, and 19 fit to better than 1 Hz. The average deviation $\bar{x}$ is 1.01, and the percent fit is 4.6. The parameters for calculating $J_{^{13}C-H}$ are reported in Table 1. Parameters for calculating the chlorine quadruple coupling constant, e^2Qq, for a series of X−Cl compounds[8,9] have also been expanded, and the revised parameters are given in Table 1. The absolute average deviation $\bar{x}$ is 1.4, and the percent fit is 1.3. Systems in which chlorine is the catimer must be treated separately from those in which it is an animer. Chlorine catimers would be combined with animers and solved for E_{ca}^*, C_{ca}^*, and T_{ca}^* for chlorine.

Table 2. Density Functional and ECT Calculated Bond Energies, D, and Bond Distances, R

	$R(Cl_3Ti-X)$		$\Delta H_D(Cl_3Ti-X)$		$-\Delta H_D((CO)_4Co-X)$	
animer, X	theor[a]	ECT[b]	theor[a]	ECT[c]	theor[a]	ECT[d]
H−	1.70	1.95	60	61	55	51
H_3C-	2.13	2.13	64	67	38	41
HO−	1.83	2.02	108	115	55	54
CH_3O-	1.86	1.95	102	93		
HS−	2.28	1.69	70	71	40	38
H_2N-	1.87	2.10	87	84	35	41
NC−	2.06	1.96	98	96	73	75

[a] From ref 11. R is the Ti−X distance, and ΔH_D, and Ti−X or Co−X bond dissociation energy. [b] Calculated with $E_{ca} = 0.132$, $C_{ca} = 0.285$, and $T_{ca} = -0.091$. [c] Calculated with $E_{ca} = 13.8$, $C_{ca} = 5.7$, and $T_{ca} = -2.5$. [d] Calculated with $E_{ca} = 2.2$, $C_{ca} = 5.0$, and $T_{ca} = 5.8$.

In the case of the $J_{^{13}C-H}$ fit, the shits are fit relative to a value of 166 for no substituent. In a similar manner, the quadruple coupling constants were calculated relative to a chlorine atom. In some cases, a reasonable estimate cannot be made of the physicochemical property with no substituent attached. When this is the case, one of the systems, e.g. that with the smallest magnitude, is selected as a reference, Rf, and the data set fit to the equation

$$\Delta\chi^{X} - \Delta\chi^{Rf} = E_{ca}^*(E_{an}^{X} - E_{an}^{Rf}) + C_{ca}^*(C_{an}^{X} - E_{an}^{Rf}) + T_{ca}^*(R_{an}^{X} - R_{an}^{Rf}) \qquad (4)$$

This procedure could also be employed to fit relative bond energies when absolute values are unknown. In this case, values found for E_{ca}^*, C_{ca}^*, and T_{ca}^* from the simultaneous equations corresponding to eq 4 can be substituted into eq 1, with reported animer parameters to provide an estimate of the absolute value. This procedure circumvents solving for the W value in reported ECW fits.

Examples of the Data Analyses. In view of the difficulty in measuring bond energies, many attempts have been made to calculate these quantities quantum mechanically or estimate them from spectroscopy. One example is selected to illustrate the utility of the ECT model in judging the results. A series of bond distances for Cl_3Ti-X molecules have been calculated by a nonlocal density functional method.[10] Theoretical results can be analyzed with the ECT model to determine whether or not they are consistent with the large experimental data base that fit with eq 1. This is accomplished by substituting the theoretical distances and animer parameters into eq 3 leading to a series of simultaneous equations that are solved to give $E_{ca}^* = 0.132$, $C_{ca}^* = 0.285$, and $T_{ca} = -0.091$. The data fit is shown in Table 2. A poor fit results. Problems are obvious in the reported[10] values for the distances. The Ti−H bond energy is calculated to be the weakest, and the Ti−H bond distance, the shortest. This is clearly inconsistent. The positive values of E_{ca}^* and C_{ca}^* also make the reported theoretical values

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(5) The revised data fits for systems reported earlier are given in: Drago, R. S. *Applications of Electrostatic-Covalent Models in Chemistry*; Surfside Scientific Publishers: P.O. Box 13413, Gainesville, FL 32605, 1994.

(6) It is essential in designing any experiment to employ atoms for which the ratios of the covalent, electrostatic, and transfer parameters are different. Many different mathematical functions will reproduce the properties of systems where only the halides or the alkali metals are varied because they differ mainly in the magnitude of the interaction and not in the relative importance of transfer, electrostatic, and bonding terms. This variation should also be considered in judging the goodness of the data fit.

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calculated for the bond distances suspect for this indicates that stronger bonding animers (larger E_{an} and C_{an}) give rise to longer distances. No one animer can be omitted from the data set to provide a meaningful fit.

The calculated bond energies for the Cl_3Ti-X system were also fit to eq 1. The trends in the reported theoretical and ECT bond energies are the same, and the average deviation in the theoretical and calculated values is 3.6 kcal mol^{-1}. If one accepts that the data fit is of comparable accuracy to expectations of the ability to calculate bond energies from theory, this error is such that an interpretation of the E_{ca}, C_{ca}, and T_{ca} values is tentative. Values of $E_{ca} = 13.8$, $C_{ca} = 5.7$, and $T_{ca} = -2.5$ result. An electrostatic interaction is indicated with an appreciable covalent contribution.

The values calculated for $(CO)_4Co-X$ bond energies[10] produce a fair fit to eq 1 with an average deviation of 3.1 (see Table 2). Tentative parameters of $E_{ca} = 2.7$, $C_{ca} = 5.0$, and $T_{ca} = 5.8$ result. The ECT interpretation of the bond strengths in the titanium and cobalt series differs from that proposed in the theoretical analysis. While both methods agree that there is more covalency in the $(CO)_4Co-X$ bond than in Cl_3Ti-X, the main difference in the bonding of the two series arises from a significantly larger transfer term in the cobalt system. With both electrostatic bonding and transfer contributing to bond polarity, it would be difficult to determine whether the titanium or cobalt bond is more polar.

IC940975I