UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

(2)

REPORT DOCUMENTATION PAGE

1b. RESTRICTIVE MARKINGS

3. DISTRIBUTION/AVAILABILITY OF REPORT
Approved for public release; distribution unlimited.

4. PERFORMING ORGANIZATION REPORT NUMBER(S)

5. MONITORING ORGANIZATION REPORT NUMBER(S)
ARO 22374.14-CH

6a. NAME OF PERFORMING ORGANIZATION
U of New Orleans

6b. OFFICE SYMBOL (If applicable)

7a. NAME OF MONITORING ORGANIZATION
U. S. Army Research Office

6c. ADDRESS (City, State, and ZIP Code)
New Orleans, Louisiana 70148

7b. ADDRESS (City, State, and ZIP Code)
P. O. Box 12211
Research Triangle Park, NC 27709-2211

8a. NAME OF FUNDING/SPONSORING ORGANIZATION
U. S. Army Research Office

8b. OFFICE SYMBOL (If applicable)

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
DAAG29-85-K-0038

8c. ADDRESS (City, State, and ZIP Code)
P. O. Box 12211
Research Triangle Park, NC 27709-2211

10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)
Interpretation and Prediction of Molecular Reactivities and Design of Synthetic Pathways, Using Electrostatic Potentials, Electric Fields and Other Properties Related to Charge Density Distributions

12. PERSONAL AUTHOR(S)
Peter Politzer

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 2/15/85 TO 8/14/88	October 7, 1988	22

16. SUPPLEMENTARY NOTATION
The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

17. COSATI CODES		
FIELD	GROUP	SUB-GROUP

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
Keywords:
Molecular Reactivities, Electric Fields, Charge Density Distributions, Energetic Molecules, Organophosphorus Systems, Bond Strengths (AW)

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

Objectives in this project have included the following:

(1) The study and elucidation of the reactive properties of certain types of energetic molecules (e.g. nitro derivatives of strained and cage systems, nitroaromatics, etc.).

(2) Developing predictive capabilities that allow the design of energetic compounds with improved performance and diminished sensitivity.

(3) The investigation of possible precursors to the target molecules, in order to help determine the most effective synthetic routes.

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20 DISTRIBUTION/AVAILABILITY OF ABSTRACT
☐ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS

21. ABSTRACT SECURITY CLASSIFICATION
Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL

22b. TELEPHONE (Include Area Code)

22c. OFFICE SYMBOL

DD FORM 1473, 84 MAR

83 APR edition may be used until exhausted.
All other editions are obsolete.

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UNCLASSIFIED

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(5) The development of new or improved quantitative techniques to help achieve the preceding objectives.

The approach has been a computational one, emphasizing the determination of structures, relative bond strengths, degrees of bond strain, energy differences, and molecular electrostatic potentials (as guides to reactive behavior). To a significant extent, we have developed ~~(under this and our previous ARO contract)~~ the analytical tools that have been used in these studies, such as the bond order formulation used to establish relative bond strengths and the bond deviation index introduced earlier as a measure of strain. Key Words)

See DD 1473

ARO 22374.14-CH

INTERPRETATION AND PREDICTION OF MOLECULAR REACTIVITIES AND DESIGN OF SYNTHETIC PATHWAYS, USING ELECTROSTATIC POTENTIALS, ELECTRIC FIELDS AND OTHER PROPERTIES RELATED TO CHARGE DENSITY DISTRIBUTIONS

FINAL REPORT

Peter Politzer

October 7, 1988

U. S. ARMY RESEARCH OFFICE

Contract Number: DAAG29-85-K-0038

Proposal Number: 22374-CH

Department of Chemistry

University of New Orleans

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APPROVED FOR PUBLIC RELEASE;

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STATEMENT OF THE PROBLEM

Our objectives in this project have included the following:

(1) The study and elucidation of the reactive properties of certain types of energetic molecules (e.g. nitro derivatives of strained and cage systems, nitroaromatics, etc.).

(2) Developing predictive capabilities that allow the design of energetic compounds with improved performance and diminished sensitivity.

(3) The investigation of possible precursors to the target molecules, in order to help determine the most effective synthetic routes.

(4) Gaining a better understanding of the factors governing the behavior of certain organophosphorus systems related to chemical defense.

(5) The development of new or improved quantitative techniques to help achieve the preceding objectives.

Our approach has been a computational one, emphasizing the determination of structures, relative bond strengths, degrees of bond strain, energy differences, and molecular electrostatic potentials (as guides to reactive behavior). To a significant extent, we have developed (under this and our previous ARO contract) the analytical tools that have been used in these studies, such as the bond order formulation used to establish relative bond strengths and the bond deviation index introduced earlier as a measure of strain.

SUMMARY OF THE MOST IMPORTANT RESULTS

A. Development of a Quantitative Measure of Relative Bond Strengths:

In seeking a detailed understanding of molecular reactive properties and stabilities, it is necessary to have some reliable quantitative means for determining how strong are the various bonds within a system. The direct quantum chemical computation of this is not feasible for molecules as large as those that are of interest to the high-energy and chemical defense programs.

As part of this project, we have developed a rapid and practical procedure for determining the relative strengths of chemical bonds. We showed, for 27 different diatomic and polyatomic molecules, that the experimentally-observed bond strengths correlate well with bond orders that we calculate with eq. (1) [1]:

$$\text{Bond Order} = 0.55747 \sqrt{k/R_e} \qquad (1)$$

k is the force constant, in mdyn/A, and R_e the equilibrium length, in A, of the bond. The force constants and bond lengths can be obtained either experimentally or computationally. Using this approach, it is now possible to evaluate and predict how the strengths of specific bonds of interest are affected by different molecular environments and substituents. An example of such an application will be discussed in the next section.

Resulting publication:

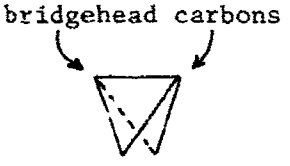
P. Politzer and S. Ranganathan, "Bond Order - Bond Energy Correlations", Chemical Physics Letters, 124, 527 (1986).

B. Analysis of Precursors in Synthetic Routes:

1. Effects of Various Substituents Upon A Strained C-C Bond:

We have analyzed how the stability and other reactive properties of a strained bond between two tertiary carbons are affected by the presence of various substituents ($-NH_2$, -NO, -NCO and $-NO_2$) on the two carbons. Derivatives involving the first three of these are possible precursors in nitration processes; thus the results of this study are directly relevant to the design of synthetic routes to the polynitration of strained hydrocarbons. We took the bond between the bridgehead carbons in bicyclobutane (I) as our model, and computed electrostatic potentials, bond deviation indices and relative bond strengths (via the bond order approach described in section A of this report) for various possible combinations of these substituents on the two carbons [2].

I



We found the bond between these carbons to be very considerably weakened by the combination of $-NH_2$ and $-NO_2$ as substituents. This can be interpreted in terms of the delocalization of the amine lone pair:

This result indicates that amines will not be effective precursors in the stepwise polynitration of strained C-C bonds, since this would go through the $-NH_2$, $-NO_2$ combination. On the other hand, the isocyanate group can also be oxidized to $-NO_2$, and we found that the -NCO, NO_2 pair produces only a relatively small weakening of the C-C bond. Thus, isocyanate precursors are clearly preferable to amines in this respect. We expanded our original study

to include the $-NH_2$, -NO combination in response to the request of Dr. G. P. Sollott (Army Research, Development and Engineering Center), who was considering working with nitroso precursors. We found that it would lead to essentially the same degree of C-C weakening as did $-NH_2$, $-NO_2$.

Resulting publication:

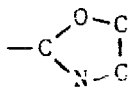
P. Politzer, G. P. Kirchenheuter, and J. Alster, "The Effects of Various Substituents upon the Properties of the Bond between the Bridgehead Carbons in Bicyclobutane", Journal of the American Chemical Society, 109, 1033 (1987).

2. Analysis of Ortho-Directed Lithiation as a Synthetic Pathway in the Polynitration of Cubane:

A potentially useful route to the synthesis of polynitro cubanes is based on the fact that certain functional groups promote lithiation of an adjacent ("ortho") carbon, which is subsequently susceptible to electrophilic attack [3,4]. We have analyzed the ortho-directing properties of several such functional groups, both in order to better understand the activating and directing mechanisms, and also to evaluate the relative effectiveness of these substituents.

(a) Focusing first on amide groups [5], we showed that they initially enhance the acidity of a hydrogen on an adjacent carbon, thus promoting its replacement by Li^+, and then interact with the lithium, thereby stabilizing the ortho-lithiated intermediate. This interaction gives rise to a channel of strongly-negative electrostatic potential leading to the lithiated carbon, which is accordingly activated toward electrophilic attack.

(b) We have also carried out a computational assessment of the relative ortho-directing powers of four other functional groups (2-oxazoline (II), trifluoromethyl (III), nitro and methyl) [6].

II  III $-CF_3$

We examined the tendencies of these substituents to interact with the lithium and produce the negative channel of approach to the ortho carbon. The ortho-activating abilities of the four groups decreased in the order listed above, with $-CH_3$ having none, as anticipated. We concluded that $-NO_2$ should have at least a moderate ortho-directing capability (which could be a very encouraging finding from the standpoint of the synthesis of polynitro derivatives) and that the effectiveness of 2-oxazoline should be similar to that of amide groups.

Resulting publications:

K. Jayasuriya, J. Alster and P. Politer, "A Computational Investigation of the 'Ortho' Directing Effect in Cubane Carboxamide" Journal of Organic Chemistry, 52, 2306 (1987);

K. Jayasuriya, J. Alster and P. Politzer, "A Comparative Evaluation of Some Ortho Directing Groups for Cubane" Journal of Organic Chemistry 53, 677 (1988).

C. Relationships Between Shock/Impact Sensitivities and Structural/Electronic Properties:

Because of the high-priority need for designing less sensitive energetic molecules, we have investigated possible relationships between shock/impact sensitivities and various structural and electronic properties. Our objective is to achieve a deeper understanding and better predictive capability for molecular sensitivity.

1. Nitramines:

The relative importance of $N-NO_2$ vs. $C-NNO_2$ bond breaking in the decomposition of nitramines is a subject of continuing investigation in many laboratories [7-11]. We have found, however, following upon important earlier studies which focused upon the role of the $N-NO_2$ linkage [8,11], that it is possible to relate shock sensitivities to the properties of this bond. A second observation has been that nitramine sensitivities can be correlated with the crystal instabilities of $-NO_2$ groups. Each of these developments shall be discussed in turn.

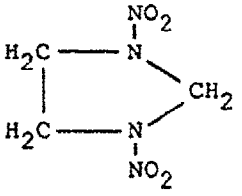
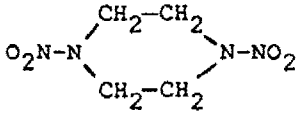
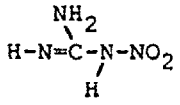
(a) Relationship of Sensitivity to $N-NO_2$ Bond Strength:

We have discovered an approximate relationship between the strengths of nitramine $N-NO_2$ bonds and their observed shock sensitivities. As a measure of relative bond strengths, we use our bond order formulation, discussed in section A of this report. The results for the seven nitramines studied show a general relationship (Table I): the molecules with higher $N-NO_2$ bond orders (and therefore stronger $N-NO_2$ bonds) tend to be the less sensitive ones.

If the $N-NO_2$ bond is of key importance in triggering nitramine decomposition, then it may be anticipated that the sensitivity will increase with the number of such "triggers" per unit weight. These data are likewise given in Table I. An immediate indication of the significance of this second parameter is seen in comparing VI and VII. They have virtually the same $N-NO_2$ bond orders, but VI has considerably more $N-NO_2$ groups per 100 grams Accordingly, we predict--correctly--that it should be more sensitive than VII.

Since the sensitivity varies directly with the number of $N-NO_2$ groups per unit weight and inversely with the $N-NO_2$ bond order, we tested the ratio of these two quantities (Table I). Overall the correlation with sensitivity is good.

Table I. Calculated Bond Orders and Experimentally-Determined Sensitivities of Some Nitramine Molecules.

	Molecules	Shock Sens.[a]	Bond Order	No. $N-NO_2$ per 100g	$\frac{N-NO_2/100g}{\text{bond order}}$
IV	RDX	~2.5	2.06	1.4	2.7
V		2.17	1.99	1.2	2.4
VI		1.64	2.03	1.1	2.1
VII	$(N\equiv C-CH_2)_2N-NO_2$	1.35	2.03	0.7	1.4
VIII		~0.90	2.16	1.0	1.8
IX	$(H_3C)_2N-NO_2$	<0.5	2.25	0.8	1.4
X	$(N\equiv C-CH_2-CH_2)_2N-NO_2$	<0.5	2.22	0.6	1.1

[a]The shock sensitivity data were kindly provided by Dr. Horst Adolph, Naval Surface Weapons Center. The numbers given in the table are the reciprocals of the distances between the explosive and the booster at which there is a 50% chance of a positive result. Thus, the larger the number in the table, the greater is the sensitivity.

(b) Relationship of Sensitivity to Crystal Instability of $N-NO_2$ Group:

When a molecule is at its equilibrium geometry in the gaseous phase, the net electrostatic force upon each nucleus, due to the electrons and all of the other nuclei, must be zero [12]. When the molecule is part of a crystal, however, its interactions with its neighbors result in certain distortions of its structure, so that the above condition no longer holds true--if the forces of only the electrons and nuclei of the molecule itself are taken into account. This net unbalanced force can be regarded as giving rise to a local destabilization.

We have found earlier that the net unbalanced force associated with the maximally destabilized $-NO_2$ group in a trinitroaromatic molecule correlates with its shock and impact sensitivities. (This work was supported by our previous ARO contract, DAAG 29-81-K-0155). Now, using crystallographic nitramine structures, we have computed the unbalanced forces in the $N-NO_2$ groups of several nitramines. Table II shows that a correlation with shock sensitivity is again observed, although unfortunately only a few data points are available. (It is difficult to find compounds for which both crystal structures and sensitivities have been determined).

Thus we have found two different approaches that are effective for correlating and predicting nitramine sensitivities; they are in terms of (1) the $N-NO_2$ bond orders, taken in conjunction with the number of $N-NO_2$ "triggers" per unit weight of compound, and (2) the net unbalanced electrostatic forces within the maximally destabilized $N-NO_2$ groups of crystalline nitramines. Method (1) has the advantage that no crystal structure data are required; accordingly it can be applied to the evaluation of proposed (not yet synthesized) target molecules.

2. Nitroaromatics

We have also completed the development (begun under our ARO contract DAAG 29-81-K-0155) of a procedure for predicting the sensitivities of trinitroaromatic compounds. We have shown that these correlate well with the positive electrostatic potential at the center of the longest $C-NO_2$ bond, as computed from the carbon and nitrogen atomic charges [13].

Resulting publication:

P. Politzer and S. Ranganathan, "Bond Order - Bond Energy Correlations", Chemical Physics Letters, 124, 527 (1986).

Table II. Calculated Unbalanced $N-NO_2$ Forces and Experimentally-Determined Sensitivities of Some Nitramine Molecules.

Molecule	Shock Sensitivity[a]	Unbalanced $N-NO_2$ Forces[b]
RDX	1.3	0.445
β-HMX	1.2	0.440
TETRYL[c] (2,4,6-trinitrophenyl-methylnitramine)	1.1	0.330
EDNA (ethylene dinitramine)	1.0	0.339
NIGU (nitroguanidine)	0.4	0.284

[a] Experimentally-measured sensitivity data were taken from A. Delpuech, "Relation entre la structure électronique moleculaire et la sensibilité au choc des explosifs secondaires", Thesis, University of Bordeaux, 1980. The figures in the table were obtained from these data, and are relative values, such that the larger the magnitude, the greater the sensitivity.

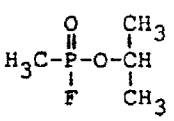
[b] The force data are in atomic units, and pertain to the maximally-destabilized $N-NO_2$ group.

[c] TETRYL contains both $C-NO_2$ and $N-NO_2$ units. Our analysis here refers only to the latter.

D. Molecules Related to Chemical Defense:

1. Sarin and Soman Analogues:

Several analogues of sarin (XI) and soman (XII) were investigated for their possible ability to elicit effective antibodies to these anticholinesterase nerve agents [14]. The key issue was whether the fluorines in sarin and soman can be replaced by some other functional group that would result in lower toxicity, so that antibodies would have the opportunity to form, but that mimics fluorine well enough that these antibodies would also show satisfactory anti-sarin and anti-soman activities. Our analysis involved a comparison of the calculated electrostatic potentials of five molecules; one (XIII) served as a sarin/soman model, while in the others the F was replaced by X, where X = CN, OH, OCH_3 or NH_2. On the basis of the electrostatic potential analysis, it was concluded that CN and OCH_3 show the greatest promise, for present purposes, as fluorine replacements.



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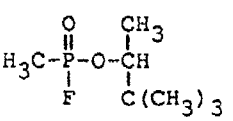

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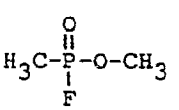


XIII

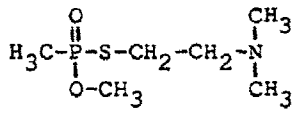
Resulting publication:

P. Politzer and K. Jayasuriya, "Computational Analysis and Comparison of Some Sarin and Soman Analogues", in Mechanism of Drug Action, Special Issue of THEOCHEM (Journal of Molecular Structure), 134, 381 (1986).

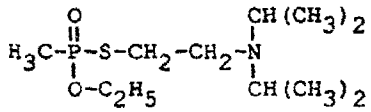
2. VX Model:

We carried out a study of XIV, taking it as a model for the organophosphorus nerve agent VX, XV [15]. The computed electrostatic potential showed major negative regions (attractive toward electrophiles) near the phosphoryl oxygen and the nitrogen, with increasingly weaker ones

in the vicinity of the alkoxy oxygen and the sulfur. On the basis of these results, taken together with our investigation of soman and sarin (see above), we suggest that a key factor in the anticholinesterase activities of these molecules is the presence of negative potentials of certain approximate magnitudes associated with the oxygens and with the sulfur in VX or the fluorine in soman and sarin. Our results support earlier speculation that the presence of the nitrogen may interfere with the metal-catalyzed hydrolysis of VX.



XIV



XV

Resulting publication:

P. Politzer, K. Jayasuriya and P. Lane,"A Study of the Reactive Properties of a VX Model Compound, as Determined by Electrostatic Potential Calculations", THEOCHEM (Journal of Molecular Structure), 34, 259 (1987).

E. Aromatic Systems:

1. Rotation of Nitro Group:

We have made a detailed examination of how the properties of nitrobenzene are affected by rotation of the nitro group by 90° from its equilibrium position in the plane of the aromatic ring [16]. This question is of considerable practical relevance, since the $-NO_2$ groups in many nitroaromatics have been forced by steric effects to undergo some degree of rotation. We have analyzed the structures and electrostatic potentials for both the equilibrium and the rotated forms of nitrobenzene. We found that there is only a very small degree of conjugation between the nitro group and the aromatic ring. Rotation of $-NO_2$ is predicted to lead to a decreased reactivity toward nucleophiles, but a slightly greater susceptibility to electrophilic attack.

Resulting publication:

P. Politzer, P. Lane, K. Jayasuriya and L. N. Domelsmith, "An Examination of Some Effects of $-NO_2$ Rotation in Nitrobenzene", Journal of the American Chemical Society, 109, 1899 (1987).

2. Nitroaromatic Molecules:

The interactions of a nitroso (-NO) substituent with an aromatic ring and with an amino group on that ring, and the manner in which these affect the overall molecular reactivity were investigated [17]. The -NO group was found to be weaker than $-NO_2$ in withdrawing electronic charge from the aromatic ring, although it definitely does deactiviate the ring toward electrophilic attack, even in the presence of an $-NH_2$ substituent. (However the directing properties of the latter are evident.) The strongest negative potentials are associated with the lone pairs of the nitroso nitrogens. Buildups of positive potential were found within the C-N-O angles, above the molecular planes of

nitrosobenzene and the nitrosoanilines; these are reminiscent of the ones associated with the C-NO_2 bonds in nitroaromatics. These positive buildups may again represent possible pathways for nucleophilic attack.

Resulting publication:

P. Politzer and R. Bar-Adon,"Computational Analysis of the Reactive Properties of Some Nitrosoaromatic Molecules", Journal of Physical Chemistry, 91, 2069 (1987).

F. Analysis of Properties Related to Chemical Reactivity:

1. Electron-Attracting Tendencies of Substituents:

We have developed a direct computational means for obtaining a quantitative measure of a substituent's total electron-attracting tendency; it is based upon the electrostatic potentials in the nitrogen lone pair regions of molecules of the type H_2N-X [18]. The magnitude of the most negative potential in this region (V_{min}), diminishes as the electron-attracting power of X increases. We computed V_{min} for 40 different substituents. A good correlation exists between V_{min} and the sum of the inductive and resonance substituent constants, $\sigma_I + \sigma_R$ (for $\sigma_R > 0$), which allows us to estimate these quantities in cases in which they are not known.

Resulting publication:

J. S. Murray and P. Politzer, "Electrostatic Potentials of Amine Nitrogens as a Measure of the Total Electron-Attracting Tendencies of Substituents" Chemical Physics Letters, accepted for publication and in press.

2. Relationship Between Charge Capacity and Hardness:

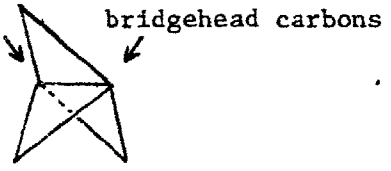
The relationship between two key properties that affect chemical reactivity has been analyzed [19]. These are the charge capacity, κ (which indicates how the electronegativity of an atom or group is modified as it gains or loses charge in forming a molecule) and the hardness, η (which has long been used as a qualitative indication of reactivity. It was found that $\kappa = 1/2\eta$, and also that κ is, for neutral atoms, a linear function of the polarizability within each of the first four rows of the periodic table.

Resulting publication:

P. Politzer, "A Relationship Between the Charge Capacity and the Hardness of Neutral Atoms and Groups", Journal of Chemical Physics, 86, 1072 (1987).

G. Strained Molecules:

We completed a study (begun under our previous ARO contract #DAAG 29-81-K-0155) of the structures, reactive properties and stabilities of [1.1.1]propellane (XVI) and bicyclo[1.1.1]pentane (XVII) [20]. XVI has rather unusual regions of relatively strong negative electrostatic potential to the outsides of the bridgehead carbons, the ones commonly described as "inverted". We propose that these carbons should be viewed as somewhat unsaturated, with no direct bonding between then. They should be attractive sites for electrophilic attack, and it is suggested that they may be reactive toward radicals as well. XVII has a less strained structure, and the C-C bonds were found to have some cubane-like character.



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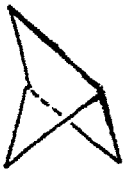

XVII

We have also computed key properties of the various $-NH_2$ and $-NO_2$ derivatives of the bridgehead carbons of XVII. These are of particular importance because they can be regarded as substituted forms of [1.1.1]propellane (XVI).

Resulting publication:

P. Politzer and K. Jayasuriya, "[1.1.1]Propellane, Bicyclo[1.1.1]Pentane and the Effects of 'Inverted' Carbons", THEOCHEM (Journal of Molecular Structure), 135, 245 (1986).

H. Calculation of Energy Differences:

We have derived a formula that makes it possible, for certain types of molecules, to calculate molecular energy differences ΔE with a high degree of accuracy from a knowledge only of the electrostatic potentials at particular nuclei [21,22]. This is an extension of earlier work performed under ARO contract #DAAG 29-81-K-0155 which removes the previous requirement that the molecules be isoelectronic. A particularly advantageous feature, which greatly improves the accuracy of the results, is that ΔE is given as a sum of terms rather than a difference.

We have also developed a procedure for accurately calculating isoelectronic energy differences through a single computation at an intermediate nuclear charge [23]. Electrostatic potentials are found to vary nearly linearly with the nuclear charge over small intervals.

Resulting publications:

P. Politzer, "Atomic and Molecular Energy and Energy Difference Formulas Based Upon Electrostatic Potentials at Nuclei" in Single-Particle Density in Physics and Chemistry, N. H. March and B. M. Deb, eds., Academic Press, New York, 1987, ch. 3.

P. Politzer and M. Levy, "Energy Differences from Electrostatic Potential Differences at Nuclei", Journal of Chemical Physics, 87, 5044 (1987).

K. D. Sen, J. M. Seminario and P. Politzer, "Z Transition State Calculations of Energy Changes and Electrostatic Potentials in Isoelectronic Atoms and Molecules", submitted to the Journal of Chemical Physics.

I. Electrostatic Effects in Bonds and in Negative Ions:

1. Chemical Bonding and Electronic Charge Distribution:

We have carried out an analysis which shows quantitatively how it is possible for the electronic charge distribution in a chemical bond to satisfy the rigorous requirement that the net electrostatic force on each nucleus be zero at equilibrium [12], without necessarily having a buildup of charge density in the internuclear region. The latter situation has been observed for a number of molecules, both crystallographically and computationally; in particular, it has been found to occur in the N-O bonds of some $-NO_2$ groups. We found at least two ways in which the required force balance can be achieved without the internuclear charge buildup that is generally regarded as characteristic of covalent bonds. These are (a) a very slight polarization of core (e.g., 1s) electronic charge, and (b) a small polarization of π charge.

2. Radii and Relative Interaction Strengths of Monoatomic Negative Ions:

Whereas the positive contributions of the nuclei dominate the electrostatic potentials of neutral atoms and postitive ions at all radial distances, those of negative ions do eventually become and remain negative as r increases. We have shown that the potential of a negative ion reaches a minimum at the radial distance r_m at which the nuclear term is exactly balanced, so that the total electrostatic potential is that due to the excess electronic charge on the ion [24]. The available evidence indicates that this uniquely-defined point can be regarded as characterizing the ion: r_m can be identified with the radius of the ion, while the magnitude of the potential at r_m directly reflects the strength of its interactions with cations (i.e. the crystal lattice energy).

Resulting publication:

K. D. Sen and P. Politzer, "Characteristic Features of the Electrostatic Potentials of Singly-Negative Monoatomic Ions" submitted to the Journal of Chemical Physics.

PUBLICATIONS AND PRESENTATIONS RESULTING FROM THIS WORK

A. Published Articles:

(1) "Computational Analysis of Some Properties Associated with the Nitro Groups in Polynitroaromatic Molecules"
Frank J. Owens, Keerthi Jayasuriya, Lars Abrahmsen and Peter Politzer, Chemical Physics Letters, 116, 434 (1985).

(2) "[1.1.1]Propellane, Bicyclo[1.1.1]Pentane and the Effects of 'Inverted' Carbons"
P. Politzer and K. Jayasuriya, THEOCHEM (Journal of Molecular Structure), 135, 245 (1986).

(3) "Computational Analysis and Comparison of Some Sarin and Soman Analogues"
P. Politzer and K. Jayasuriya, in Mechanism of Drug Action, Special Issue of THEOCHEM (Journal of Molecular Structure), 134, 381 (1986).

(4) "Bond Order - Bond Energy Correlations"
P. Politzer and S. Ranganathan, Chemical Physics Letters, 124, 527 (1986).

(5) "Atomic and Molecular Energy and Energy Difference Formulas Based Upon Electrostatic Potentials at Nuclei"
P. Politzer in Single-Particle Density in Physics and Chemistry, N. H. March and B. M. Deb, eds., Academic Press, New York, 1987, ch. 3.

(6) "A Study of the Reactive Properties of a VX Model Compound, as Determined by Electrostatic Potential Calculations"
P. Politzer, K. Jayasuriya and P. Lane, THEOCHEM (Journal of Molecular Structure), 34, 259 (1987).

(7) The Effects of Various Substituents Upon the Properties of the Bond Between the Bridgehead Carbons in Bicyclobutane"
P. Politzer, G. P. Kirschenheuter and J. Alster, Journal of the American Chemical Society, 109, 1899 (1987).

A. Published Articles (Continued):

(8) "A Relationship Between the Charge Capacity and the Hardness of Neutral Atoms and Groups"
P. Politzer, Journal of Chemical Physics, 86, 1072 (1987).

(9) "A Computational Investigation of the 'Ortho' Directing Effect in Cubane Carboxamide"
K. Jayasuriya, J. Alster and P. Politer, Journal of Organic Chemistry, 52, 2306 (1987).

(10) "Computational Analysis of the Reactive Properties of Some Nitroso-aromatic Molecules"
P. Politzer and R. Bar-Adon, Journal of Physical Chemistry, 91, 2069 (1987).

(11) "An Examination of Some Effects of $-NO_2$ Rotation in Nitrobenzene"
P. Politzer, P. Lane, K. Jayasuriya and L. N. Domelsmith, Journal of the American Chemical Society, 109, 1899 (1987).

(12) "Energy Differences from Electrostatic Potential Differences at Nuclei"
P. Politzer and M. Levy, Journal of Chemical Physics, 87, 5044 (1987).

(13) "A Comparative Evaluation of Some Ortho Directing Groups for Cubane"
K. Jayasuriya, J. Alster and P. Politzer, Journal of Organic Chemistry 53, 677 (1988).

B. Articles Accepted for Publication and In Press:

(14) "Electrostatic Potentials of Amine Nitrogens as a Measure of the Total Electron-Attracting Tendencies of Substituents"
J. S. Murray and P. Politzer, Chemical Physics Letters, accepted for publication and in press.

C. Articles Submitted for Publication:

(15) "Z Transition State Calculations of Energy Changes and Electrostatic Potentials in Isoelectronic Atoms and Molecules"
K. D. Sen, J. M. Seminario and P. Politzer, submitted to Journal of Chemical Physics.

(16) "Characteristic Features of the Electrostatic Potentials of Singly-Negative Monoatomic Ions"
K. D. Sen and P. Politzer, submitted to the Journal of Chemical Physics.

D. Presentations:

(1) Working Group Meeting on "Synthesis of High Energy Density Materials", U.S. Army Armament Research and Development Command, Dover, NJ, June, 1985.

(2) Working Party on Explosives, U.S. Army Armament Research and Development Center, Dover, NJ, July, 1985.

(3) Energetic Materials Division, U.S. Army Armament Research and Development Center, Dover, NJ, August, 1985.

(4) Scientific Conference on Chemical Defense Research, Sponsored by Chemical Research and Development Center (Aberdeen Proving Ground, MD), November, 1985.

(5) Working Group Meeting on Synthesis of High Energy Density Materials, U.S. Army Armament Research, Development and Engineering Center, Dover, NJ, May, 1986.

(6) Gordon Conference on Electron Distributions and Chemical Bonding, Plymouth, NH, July, 1986.

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None.

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