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Annual Progress Report Contract N° DA-91-591-EUC-1897

Photo-activated Production of Free Radicals from Diatomic Molecules After Adsorption on Metallic Surfaces

685 600

by C. M. MOSER, Institut Pasteur - PARIS 15e

The research reported in this document has been made possible in part by the support and sponsorship of the U.S. Department of the Army through its European Research Office.

Period Covered : 1 November 1961 - 30 October 1962

SUMMARY

This year's activities have been mainly centered in two fields : (a) atomic hyperfine structure spectra calculations and (b) electronic structure of diatomic molecules. A smaller effort has been directed towards the study of chemical reactivity in alternant and non-alternant hydrocarbons. This has been the principal activity of one of our visitors, Mrs J. Kaufman from the RIAS division of the Martin Aircraft Company, Baltimore.

Under (a) we have now completed calculations for the atomic hfs spectra constants for the following states : ^4S of N^{14}, $^3P_{3/2}$ and $^3P_{1/2}$ of B^{11}, $^3P_2$ and $^3P_1$ of O^{17} and $^3P_{3/2}$ and $^3P_{1/2}$ of F^{19}. A technical report was issued last year for N^{14} and this year for B^{11} and O^{17}. So in this annual report we will concentrate on making a survey of these results and giving the results for F^{19}. This work fits in well with other work going on in other laboratories - in particular the Ordnance Materials Research Office at Watertown Arsenal. It is gratifying that the kind of wave functions which can now be calculated from currently available machine programs are certainly adequate to give qualitative agreement with experiment.

Under (b) we have now completed our study of all known electronic excited states of carbon monoxide. Previously we have shown that the states which arise from valence state excitations are well accounted for by LCAO-MO-SCF functions. Now we have shown that the Rydberg molecular

states can be equally well explained by the same kind of wave function using an expanded basis set. This work has been reported in a brief technical report which represents a paper delivered before the International Symposium on Molecular Structure which was held in Tokyo in September, 1962.

With the results now in hand for CO it should be possible to examine the spectra of other diatomic molecules in considerable detail. While quantitative data can only be obtained from experiment, good qualitative information can now be readily found from calculations. It is entirely possible that the calculations can complement experimental data which either has not or cannot be studied in great detail.

In addition to the study of electronic excited states, we have calculated (using different basis sets) the dipole moment of CO and the gradient of the electric field at the oxygen nucleus in CO both for the $X^1\Sigma^+$ ground state. The dipole moment of the ground state has been deduced from an analysis of microwave spectra and it is likely to be very accurate. But this method does not seem to be applicable to excited states or to ions. New methods have been developed which give rather surprising results, and it will be most important to develop techniques of accurate calculation of the dipole moment which has been one of the most difficult quantities to obtain with any assurance. The experimental difficulties of determining the gradient of the electric field are well known even though this kind of experiment should be one of the most fruitful for the discussion of the chemical bond. Happily it appears that stable numerical results can be much more easily obtained for q than for the dipole moment.

Considerable work has been done on the excited electronic states of NO. An adequate representation of the experimental data is difficult for two reasons : (a) there is clear experimental evidence in this molecule that two states of the same symmetry "cross" ; (b) the formal problem of writing down the SCF equations is complicated by the fact that as there are π orbitals both quadruply and singly occupied, there are in fact two compled SCF equations which should be solved. Good progress has been made though some work remains before the work will be ready for publication.

One of our visitors during the summer was Dr. K. D. Carlson of the Case Institute of Technology. Dr. Carlson is interested in the calculation of the heat of dissociation of TiO which is an important refractive material and has a high enough vapor pressure to make calculations as a diatomic molecule of value. Very little is known about the molecule experimentally ; the symmetry of the ground state is not even known with any certainty. Some preliminary calculations have been carried out using one exponent per atomic orbital. This is certainly an insufficient basis but when one considers that even so each calculation takes 3-4 hours on an IBM 704 it will be realized that a wide search for the best function in the simplest basis will be desirable before proceeding to larger basis sets.

One of our visitors during the year was Dr. J. P. Auffray of the AEC Computing Center, New York University. Dr. Auffray has developed a method for an accurate calculation of the ground state wave function for helium. Contrary to earlier ways of calculating an accurate wave function of two electron systems , this method can probably be extended to somewhat larger atoms, though with each additional electron the additional computational effort is considerable.

I Scientific Work

a) Calculation of atomic hyperfine spectra constants.

We should perhaps first of all recall the methods which we have used to calculate the hyperfine constants. For a given set of analytic basis functions we can, using a program written for the IBM 704 by Dr. R. K. Nesbet and, in part, Dr. R. Watson, calculate either the usual Hartree-Fock orbitals or the spin polarized HF orbitals.

As it is well known the HF orbitals are themselves not adequate to represent the exchange polarization effects which play an essential role in the hyperfine spectra, we construct a configuration interaction function which includes the HF function plus all possible single excitations. If it has been recognized for sometime that the introduction of exchange polarization effects for the s electrons was necessary, recent experimental work on the J excited states of O^{17} and F^{19} by Dr. S. Harvey at the Clarendon has indicated that the same sort of mechanism is necessary for the p electrons also.

This complicates matters, for it increases materially the size of the configuration interaction matrix. If, in general, each $s \rightarrow s$ excitation gives rise to two functions, it can easily be arranged that one of these has a zero matrix element with the ground state for both the total Hamiltonian and the Fermi contact term. But for each p. ,p excitation this cannot be done. If the problem of determining the eigenfunctions of S^2 and L^2 for a given configuration is one fo the major obstacles to the study of atomic structure, the classical methods becoming quickly unmanageable, Dr. R. K. Nesbet has recently published a very convenient method to find the eigenfunctions and which can then be manipulated in a very straightforward method to obtain the matrix elements.

Using spin polarized functions to introduce spin polarization in the p electrons also is more complicated. Until the recent work mentionned above on O^{17} one might have thought that the proper SP function to discusss S - polarization in O^{17} would be the type where the orbitals S^{α} are solutions of a different equation than S^{β} , but that all the p orbitals are solutions of the same equation. If then we compare the value of a_s obtained from the one where not only the s orbitals but also the p orbitals are solutions of different equation, then we find a very different value to a_s . There is the question of course whether there will be only one or several p^{α} orbitals and like wise for the p^{β} orbitals but whether one uses one or several equations for p^{α} (and P^{β}) is only a second-order effect. The fit to the experimental data is made with two (r^{-3}) integrals so the polarization of the p orbitals is essential. But this polarization of the p orbitals has a considerable effect on the polarization of the s orbitals.

As is well known the spin polarized functions are not in general eigenfunctions of S^2 and in some cases are not eigenfunctions of L^2 either. Thus if one wishes to find a function which corresponds to a definite spectroscopic state then it is necessary to project out the desired state. Whether the unprojected or projected function better corresponds to the physically observed phenomenon is a difficult problem. In the particular case where the spin polarized function is an eigenfunction of L^2 Marshall has proposed that the magnetic hyperfine constant calculated should be "better" calculated from the spin polarized function than form the function obtained from the projection of the spin polarized function. This argument is rather complicated but essentially it comes down to the idea that if in projection. one eliminates the unwanted functions, far more important one is changing the normalization of the function desired so that the overall result in projection is unfavorable. In fact there is evidence to show that the hyperfine constant of the ^2S state of Li calculated from the spin polarized function is in better agreement with experiment than the hyperfine constant calculated form the porjection of this spin polarized function to obtain the ^2S state (Sachs). But at the meeting on "Recent Developments in Quantum Chemistry" which was held at Hakone National Park, Japan, in September, 1962, Ishiguro and his co-workers have found that if the parameters in the projected functions are not those of the spin polarized function but are chosen such as to minimize the energy of the projected function, then the hyperfine constant calculated from this function which is an eigenfunction of S^2 is in better agreement with experiment than the constant obtained form the spin polarized function.

Be this as it may, if we use spin polarized functions where both s and p orbitals are polarized, then the calculated constants are much larger than those observed. The rigorous projection with respect to L^2 and S^2 is a formidable task for two reasons : (1) the projection gives rise to a very large number of determinants ; (2) the calculation of the matrix elements between these determinants is complicated by the fact that the spin polarized orbitals, being solutions of different SCF equations are not orthogonal. So, without a machine program, which we do not at present possess, it really is necessary to use some approximations in carrying out the projections.

In Technical Report N° I we gave a simple procedure for calculating the constants from the projected functions of O^{17}. More recently in our work on F^{19} we have been reinvestigating the problem in more detail. The final results are not yet quite ready but we can give the general approach here. We have assumed that the overlap between orbitals [illegible] = 1 (where the prime refers to orbitals found from a different equation than the unprimed) and [illegible] = 0 . On a typical calculation these assumptions are really quite accurate for s orbitals and still seem to be of the right order of magnitude for p orbitals. In this way we can reduce considerably the number of determinants which appear in the projection.

With those that remain it is not too difficult to calculate the hyperfine constants and preliminary results indicate that the numerical values obtained by our very approximate procedure are in very close agreement with the new results.

There remains one problem which is not yet solved. Our whole procedure is based on minimization of the energy of the function used to calculate the constants with respect to the parameters. There is every reason to believe these would not be the same for the spin polarized as for the projected function. Even if a proper extended Hartree-Fock function is beyond the present possibilities, that would not mean we could not calculate the energy of our projected function as a function of the parameters. Unfortunately the use of a two electron operator is much more complicated than the single electron operators for $\overset{\text{in}}{/}$the multideterminant function for the determinants are not orthogonal.

The results for the hyperfine constants B^{11}, O^{17} and F^{19} are summarized in Tables I, II and III.

b) "Best" single exponents for Ti atom

In connection with work on TiO which has been started with Dr. K. D. Carlson we have been interested in the "best" exponents for the ^3F state of Ti using only one exponent per orbital. In fact Watson has given an analytic basis set for the HF representation of the atom. This is so large that if we used in addition one of our extended basis sets for oxygen the calculation for the TiO molecule, might well take 24 hrs ! Thus these was every reason to vary the single exponent basis for Ti . These calculations take only 20 - 30 sec. a piece so we have been able to do quite a few. The results here are incomplete because the possible variation in the set 1s , 2s , 3s , 4s , 2p , 3p , and 3d is enormous. Still a few conclusions seem clear and are particularly interesting in comparison with the first row atoms.

Thus : (a) The difference in energy given by Slater exponents and the HF energy is roughly of the same order for Ti as for the first row elements. The best exponents that we have found give a considerably better energy than that found from Slater exponents ; (b) There is not a uniquely defined set which will give the same energy. There seems to be several very different sets of exponents which all give about the same "best" energy.

c) Electronic States of Carbon Monoxide

During this year we have completed our work on the calculation of potential curves for the molecular Rydberg states of carbon monoxide. This work is the subject of Technical Report N° 2.

Briefly here we shall recall that we have calculated these states from a configuration interaction built on occupied and virtual LCAO-MO-SCF orbitals determined for the $X\,^1\Sigma^+$ ground state. As basis orbitals Is , 2s , 2p , 3s and 3p atomic functions on each center were used with Slater exponents for these atomic functions. The results for the Rydberg states are summarized in Table IV.

The calculation of potential curves for both valence excitation and molecular Rydberg states of CO was one of the chief aims of the original contract proposal.

We can now summarize our results as follows : It seems perfectly possible with relatively simple calculations to qualitatively describe not only the valence excited states but also the Rydberg molecular states. And of course these calculations use no experimental data whatsoever. Perhaps some stress needs to be put on the work qualitative. Precise quantitative data must still be found from experiment, but, of course, no one would suggest quantum mechanical calculations are ready to displace experiments. Still, the calculations can be an extremely useful adjunct of experiment. Occasionally the experimental data cannot or has not been adequately interprotated. A state has been assigned one symmetry when in fact it has another. Or a force constant has been established which is likely off by a factor of 4 or 5. The qualitative description may be very useful in itself for many needs and this one should be able to get from experiment. Particularly useful will be the qualitative estimation of the energies of different states as yet unobserved or in the process of investigation.

d) <u>Electronic States of Nitric Oxide</u>

Nitric oxide presents a particular interest for theoretical study on two accounts : (1) There is the formal problem because this is a molecule with an old number of electrons ; (2) In the observed spectrum there is a clear example of two states of the same symmetry ($^2\pi$) which "cross", i.e. the perturbations to the vibrational structure of the states in the region where they are close together is no more than is observed between two states of different symmetry.

The formal problem arises form the fact that as one π molecular orbital is quadruply occupied and one is singly occupied the

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rigourous SCF procedure would be too have two coupled SCF equations to calculate these two orbitals. But as we are using a program due to Dr. R. K. Nesbet to calculate the SCF orbitals which necessitates the use of only one equation per symmetry then a compromise had to be sought.

Miss Kreiss has written a Third Cycle Thesis in the Sorbonne on the use of the Hamiltonian for the quadruply occupied orbitals only. She found that the SCF orbitals thus obtained were rather unsatisfactory to describe the two $^2\pi$ states mentionned above. Miss Kreiss developed a method for the transformation of the orbitals which were much better for the description of the excited states but still the method was rather cumbersome.

Miss Carnam spent the summer months reinvestigation the problem. In particular she used the Hamiltonian proposed several years ago by Dr. Nesbet according to what he called "Symmetry and equivalence restriction". Even though we do not know what the rigorous SCF orbitals are we can dalculate how closely the orbitals which we have obtained satisfy certain self-consistent conditions. The orbitals obtained satisfy these conditions in a very satisfactory manner.

There remains to calculate the energies of excited states of other symmetries.

e) Comparison of Various Techniques for Calculation of Localization Energies for Alternant and Non-Alternant Hydrocarbons.

Among the various indices for chemical reactivity of π systems, the relation of localization energies to the reactivities toward substitution has been considered to be a valid criterium for the evaluation of reactivities. However a fundamental problem arose when one made a comparison between localization energies calculated by the Hückel or the Pariser-Parr (without iterations) methods. While the relation between localization energies calculated by the two methods for alternant hydrocarbons is approximately linear, preliminary calculations seemed to indicate that for non-alternant hydrocarbons not only a non-linear relationship was found but it even might be in the opposite direction (Fukui). For the alternant hydrocarbons benzene, naphthalene, and anthracene a linear relationship between localization energies calculated by the Hückel method and by the Pariser-Parr-Pople SCF approximation.

In the present study the calculation of the localization energies of five alternant and eight non-alternant cyclic hydrocarbons using the techniques of Hückel, Pariser and Parr and SCF Pariser-Parr was undertaken in an attempt to elucidate more clearly the variation in localization energies of non-alternant molecules as a function of the method used. The results should be of importance in the theoretical interpretation of chemical reactivities, in particular if one were to extend the study of systems which contain heteroatoms.

The calculations were carried out on the IBM 7090 using a program written by Dr. G. Bessis and Dr. O. Chalvet.

Our results confirm those obtained by Fukui and his collaborators. For alternant hydrocarbons similar electrophilic and nucleophilic potential barriers are found from either the Hückel Pariser-Parr methods. We have also calculated the potential barriers using SCF orbitals (calculated in Pariser-Parr-Pople approximation) and have found the same results.

For non-alternant hydrocarbons the results obtained by the different methods are not always in the same order. Some results which we have obtained are collected in Table V (J. Kaufman).

II Visits, Seminars, International Symposium

The scientific work given in this progress report has been the subject of papers delivered before :

- 1) the Theoretical Chemistry Group (Cambridge).
- 2) the Chemistry Department (University College, London).
- 3) the Clarendon Laboratory (Oxford).
- 4) the Mathematical Institut (Oxford).
- 5) Conference on Recent Developments in Theoretical Chemistry (Hakone National Park, Japan).
- 6) International Symposium on Molecular Structure (Tokyo).

III Personnel

During the contract period the principal investigator spent nearly full time on the project. Without expense to the contract the research has benefited from the nearly full time activity of :

- Dr. Helene Lefebvre-Brion and Mrs. N. Bessis.
- Dr. Yamazaki was full time on the project November 1, 1961 to April 30, 1962 (about 1 200 hours).
- Dr. J. Kaufman was full time on the project May 1, 1962 to October 30, 1962 (about 1 200 hours).
- Miss D. Carnam was full time on the project June 1, 1962 to August 31, 1962 (about 600 hours).
- Miss Kreiss was part time on the project November 1, 1961 to September 30, 1962 (about 1 100 hours).
- Dr. K. D. Carlson was a visitor to the project from June 15, 1962 to August 15, 1962 (about 250 hours).
- Dr. J.P. Auffray was a visitor to the project from May 1, 1962 to June 15; 1962 (about 150 hours).

IV Materials, Property, Etc...

No property has been acquired and the only expendable materials obtained have been included in overhead (Stationery, etc...).

Table I

Magnetic hyperfine constant for F^{19} (Mc/sec)

constant	HF function	CI		SP		EXP
		2r.f."p"	3r.f."p"	2r.f."p"	3r.f."p"	
$\langle X_l \rangle$	2537	2534.8	2588.2	2484.6	2809	2452.7
$\langle X_d \rangle$	-507.4	-480.8	-485.4	-496.9	-473	-544
$\langle X_c \rangle$	0	-18.05	-10.79	213.7	315.3	101.3
a(3/2)	2029.6	2036	2092	2201.4	2651.9	2010
a'(3/2)	-634.3	-487	-512	-407.4	-498.3	-445
a(1/2)	10.148	9885	10041	9724.8	10034.1	10.244
E(au)	-99.407505	-99.410	-99.410	-99.4693	-99.4614	-99.804

Parameters

s $\begin{cases} Z_1 = 8.76 \\ Z = 2.13 \end{cases}$

2p $\begin{cases} 5.954 \\ 3.068 \\ 1.752 \\ 0.786 \end{cases}$

3p 4.17

$$\langle X_l \rangle = \langle \tfrac{3}{2}\,\tfrac{3}{2} | \sum_i \frac{l_{zi}}{r_i^3} | \tfrac{3}{2}\,\tfrac{3}{2} \rangle / \mu\,\beta_e\,\beta_n$$

$$\langle X_d \rangle = \langle \tfrac{3}{2}\,\tfrac{3}{2} | \sum_i \frac{3\cos^2\theta_i - 1}{r_i^3} S_{zi} | \tfrac{3}{2}\,\tfrac{3}{2} \rangle / \mu\,\beta_e\,\beta_n$$

$$\langle X_c \rangle = \langle \tfrac{3}{2}\,\tfrac{3}{2} | \sum_i \delta(\vec{r}_i) S_{zi} | \tfrac{3}{2}\,\tfrac{3}{2} \rangle / \frac{16\pi}{3}\,\mu\,\beta_e\,\beta_n$$

Table II

Magnetic Hyperfine constants for ^2p states of B^{11} (Mc/sec)

	Analytic(a) HF function	Numerical HF function	CI (a) function	Analytic (a) UHF function	Analytic (b) UHF function	Numerical UHF function	Projected (a) UHF function	Projected (b) UHF function	Experience
a_s	0	0	- 3.8	5.1	- 5.9	8.2	1.7	- 1.97	0.11
a_p	70.8	70.74	70.3	71.25	71.22	71.31	71.25	71.22	73.24
$a_{3/2}$	70.8	70.74	67α	76.35	63.32	79.5	72.95	69.25	73.35
$a_{1/2}$	354.0	353.6	357.8	351.15	362.0	343.35	354.55	358.07	366.09
$E_{\varepsilon u}$	- 24.5285	- 24.53	- 24.529	- 24.529	- 24.529				- 24.66

Analytic basis functions are for 2p (Z = 0.3662 ; 1.3946 ; 2.7692 ; 7.3539)
from the fit of D.A. Dalgarno (private communication)
The "s" basis orbitals are (a) 1s, 2s, 3s (Z = 5.0 ; 1,14)
(b) 1s (Z = 3.9469 ; 4.3308 ; 7.605)
2s (Z = 1.1571 ; 2.0387 ; 8.682)

The numerical constant $\frac{2\beta_\eta\beta_e}{I}$ = 171.0113 a_o^3 (Mc/sec.)

Table III

Hyperfine constants for ^3p states of O^{17} *

	Analytic	UHF only	Approximations EHF TypeI			Approximations EHF, Type II					
	HF function	s spin-polarized	UHF	Proj.UHF	CI	UHF type IIa	Proj.UHF Type IIa	UHF Type IIb	Proj.UHF Type IIb	CI	Expérience
a_2(Mc/sec)	-215.7	-235.7	-235.3	-220	-212	234.2	-213.3	-236.5	-219.8	-216.1	-210.569 $\pm$ 0.003
a'_2	-145.3	-134.3	-115.9	-127.6	-129.4	-115.4	-126.9	-117.3	-127.5	-131.9	-126.6 $\pm$ 1.4
a_1	0	-19.5	-34.1	-9.2	-2.4	-34.1	-3.1	-23.3	-8.6	-3.3	4.739 $\pm$ 0.009
a'_1	-146.8	-115.2	-81.2	-102.7	-109.4	-77.9	-101.1	-76.3	-102	-113.1	-91.3 $\pm$ 1.4
E (au)	-74.8083	-74.8096	-74.8117		-74.8129	-74.8117		-74.8119		-74.8132	-75.105
$\langle r^{-3}\rangle / 10^{25} cm^{-3}$	3.36	3.36	3.13	3.13	3.10	3.11	3.11	3.13	3.13	3.16	3.06
$\langle r^{-3}\rangle'$	3.36	3.36	3.13	3.28	3.26	3.26	3.23	3.24	3.29	3.30	3.46
$\langle r^{-3}\rangle''$	3.36	3.36	3.13	3.13	3.10	3.11	3.13	3.03	3.12	3.08	?
a_s (Mc/sec)	0	-19.5	-34.1	-17.1	-11.4	-34.1	-17.1	-34	-17	-11.5	-13

* Analytic basis functions are for 2p (ζ = 1.4107 ; 2.7489 ; 5.9169)
for s (ζ = 7.8 ; 1.9)

The numerical constant $\frac{2\beta_n\beta_e}{I}$ = -72.24933 $a_o 3$ Mc/sec.

TABLE IV

Molecular Constants for Some Electronic States of CO

Electronic state	r_e (A°)		k (10^5 dyne cm^{-1})		energies from $X^1\Sigma^+$ (ev)	
	observed (a)	calculated	observed (a)	calculated	observed (a)	calculated
$B^1\Sigma^+$	1.12	1.18_0	19.07	18.64	10.77	10.61
$C^1\Sigma^+$	1.125	1.18_5	20.01	18.18	11.39	11.07
$E^1\Sigma^+$		1.18_8	20.03	17.71	11.52	12.34
$b^3\Sigma^+$	1.088	1.17_3	21.25	19.13	10.39	10.37
$c^3\Sigma^+$	1.121	1.18_7		18.08		11.54
$F^1\pi$		1.17_6		18.75	12.36	11.24
$G^1\pi$		1.20_3	5.29	16.10	13.05	13.09
$^3\pi_b$		1.17_2		19.55		11.27
$X^1\Sigma^+$	1.128	1.17_4		20.10		

(a) Most of the data is taken from G. Herzberg, Molecular Spectra and Molecular Structure ; Spectra of Diatomic Molecules (D. Van Nostrand Co, Princeton) 2nd edition.

(b) This state is the second state of symmetry $^3\pi$.

Table V

Electrophilic Potential Barrier Energies

Alternant Hydrocarbons

Molecule	Position	Hückel (β)	P and P_o[x] (ev)	P and P final[xx] (ev)
Benzene	1	2.5359	-25.7287	-25.7147
Naphthalene	2	2.4796	-25.3642	-25.1991
	1	2.2986	-24.8040	-24.6428
Anthracene	2	2.0131	-23.6898	-23.5019
	13	2.4227	-25.1241	-24.8401
	14	2.305	-24.4728	-24.2134
Biphenyl	3	2.4422	-25.0937	-24.9402
	4	2.5442	-25.7448	-25.5130
	5	2.4000	-25.0379	-24.8889

Non Alternant Hydrocarbons

Molecule	Position	Hückel (β)	P and P_o[x] (ev)	P and P final[xx] (ev)
Fluoranthene	1	2.3411	-24.5552	-24.3460
	2	2.5026	-25.4285	-25.0615
	3	2.4655	-24.8113	-24.6876
	6	2.3710	-24.5103	-24.4359
	7	2.4347	-24.7494	-24.6101
Fulvene	1	2.2298	-24.6680	-24.9168
	5	2.2396	-24.7227	-24.8556
	6	2.0018	-23.8035	-23.9856

x 0^{th} iteration

xx SCF convergence