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TECHNICAL REPORT ARBRL-TR-02109

SINGLE-ELECTRON AND EXCITATION ENERGIES
BY THE NON-MUFFIN-TIN X- α METHOD

D. A. Ringers
J. B. Danese

October 1978

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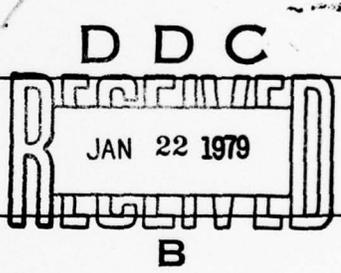
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muffin-tin (MT) calculations while taking less time than comparable total energy calculations.

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I. INTRODUCTION

The energetics of the propellant are of fundamental importance in ballistics technology. The amount of energy which can be utilized to impart thrust to the projectile depends upon the reaction mechanism of the particular propellant. As the propellant is activated, its deflagration proceeds along certain reaction paths changing from one energetic state to another. The energy obtainable from a state-to-state transition, as well as the time a given transition takes, may be calculated by quantum chemical means. In order to determine the energy one may use the "transition state" procedure which relates total energy differences to differences in electronic orbital energies (single-electron eigenvalues). This procedure is valid for any states which are describable in a single-electron picture; that is, when the effects upon a single electron are, to a good approximation, due to a potential field which is an average field generated by all the other electrons taken in their entirety.

In this paper we describe a method for calculating single-electron eigenvalues by the X- α method with non-muffin-tin (NMT) corrections^{1,2}. We calculate and compare ionization energies using the X- α transition state method (referred to as NMT or NMT-transition) and the method of total energy differences (referred to as Δ SCF), both with NMT corrections, for the molecules CO, NO, SN, and H₂CO. The results for the NO and SN molecules using the method of total energy differences have been previously reported³. Substantial improvement is obtained over muffin-tin (MT) calculations for the NMT X- α total energy calculations. The results compare very well with experiment and with other methods which have been advanced for calculating X- α transition-state energies such as the overlapping-spheres (OS) method⁴, the discrete-variational method (DVM)⁵, and the method of Sambe and Felton⁶. The present NMT X- α method is comparatively economical and can be extended to larger molecules, just as was the original multiple-scattering X- α (MSX- α) method in the muffin-tin approximation (referred to MT-transition). The work reported here was done primarily to test the method and to determine its usefulness.

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II. THEORY

The relationship between the MT approximation and the NMT corrections for the X- α total energy and eigenvalues has been described elsewhere¹. In essence, the correction to the eigenvalues is obtained as a first-order perturbation correction to the MT one-electron eigenvalues. The perturbation is the difference between the total one-electron potential obtained using the orbitals of the MT one-electron equation [the set (\bar{u})] and the MT average of the potential obtained using the MT density. In what follows a bar (-) over a quantity will indicate a MT function and a Δ preceding a symbol will indicate a NMT function. The X- α one-electron differential equation for the orbital u_i of the eigenvalue ϵ_i is

$$[-\nabla^2 + v([\rho], \bar{r})] u_i(\bar{r}) = \epsilon_i u_i(\bar{r}). \quad (1)$$

The usual MT X- α one electron equation is

$$[-\nabla^2 + \bar{v}([\bar{\rho}], \bar{r})] \bar{u}_i(\bar{r}) = \bar{\epsilon}_i \bar{u}_i(\bar{r}). \quad (2)$$

Note the different functional dependences upon ρ in the two equations (ρ versus $\bar{\rho}$). As is shown in reference 1, the MT one-electron potential is a MT function and also depends functionally on $\bar{\rho}$. The X- α potential consists of the three types of contributions

$$v([\rho], \bar{r}) = v_{Ne}(\bar{r}) + v_c([\rho], \bar{r}) + \frac{4}{3} c_\alpha \rho(\bar{r})^{1/3}, \quad (3)$$

where the first term is the nuclear-electron potential, the second is the electron-electron Coulomb interaction potential, and the last is the X- α approximation to the exchange potential. Taking the difference of the two potentials of Eq. (1) and Eq. (2), we get for the perturbation

$$\Delta v(\bar{r}) = \Delta v_{Ne}(\bar{r}) + \Delta v_c(\bar{r}) + \Delta v_{exc}(\bar{r}), \quad (4)$$

where the first two terms are the NMT analogues of the first two terms in Eq. (3), and Δv_{exc} is given

$$\Delta v_{exc}(\bar{r}) = \frac{4}{3} c_\alpha (\rho(\bar{r})^{1/3} - \bar{\rho}(\bar{r})^{1/3}), \quad (5)$$

(here $c_\alpha = -9\alpha(3/8\pi)^{1/3}$ and α is the exchange parameter⁷). The definition of the Coulomb potential of Eq. (1) is, in rydbergs,

7. K. Schwarz, Phys. Rev. B5, 2466 (1972).

$$v_c([\rho], \vec{r}) = \frac{2\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}' \quad (6)$$

We may break up ρ and v_c into their MT and NMT parts,

$$\rho(\vec{r}) = \bar{\rho}(\vec{r}) + \Delta\rho(\vec{r})$$

and

$$v_c([\rho], \vec{r}) = \bar{v}_c([\bar{\rho}], \vec{r}) + v_c([\bar{\rho}], \vec{r}) + \bar{v}_c([\Delta\rho], \vec{r}) + v_c([\Delta\rho], \vec{r}). \quad (7)$$

Hence Δv_c of Eq. (4) is

$$\Delta v_c(\vec{r}) = \Delta v_c([\bar{\rho}], \vec{r}) + \bar{v}_c([\Delta\rho], \vec{r}) + \Delta v_c([\Delta\rho], \vec{r}). \quad (8)$$

With this definition the first order perturbation $\Delta\epsilon_i$ to the MT eigenvalue ϵ_i is given by

$$\Delta\epsilon_i = \int \left\{ \Delta\rho_i(\vec{r}) \Delta v_{Ne}(\vec{r}) + \Delta\rho_i(\vec{r}) \Delta v_c([\bar{\rho}], \vec{r}) + \bar{\rho}_i(\vec{r}) \bar{v}_c([\Delta\rho], \vec{r}) \right. \\ \left. + \Delta\rho_i(\vec{r}) \Delta v_c([\Delta\rho], \vec{r}) + \rho_i(\vec{r}) \Delta v_{exc}(\vec{r}) \right\} d\vec{r}. \quad (9)$$

Here use has been made of the fact that the integral of a MT function with a NMT function is always zero(1). (The exchange part is not of this form as may be seen by examining the definition of Δv_{exc} , Eq. (5).

It is, however, a three-dimensional integral.) The third term of Eq. (9) may be rearranged in a different and computationally more convenient way:

$$\int \bar{\rho}_i(\vec{r}) \bar{v}_c([\Delta\rho], \vec{r}) d\vec{r} = \int \Delta\rho(\vec{r}) \Delta v_c([\bar{\rho}_i], \vec{r}) d\vec{r}. \quad (10)$$

With this rearrangement all the integrals of Eq. (9) are three dimensional except the last one. Being three dimensional, they are amenable to evaluation using three dimensional Gaussian integration as described in reference 2. The last integral is basically a six dimensional integral, which for a general molecule cannot be reduced further, (although certain simplifications do occur for highly symmetric molecules). As part of this study we will determine the importance of this term in $\Delta\epsilon_i$.

The ionization energies are calculated here using the well-known transition state formulated for the X-alpha theory by Slater, et al.^{8,9}, in which the occupation of the level in question is reduced by one-half

8. J.C. Slater and J.H. Wood, Intern. J. Quan. Chem. 48, 3 (1971); J.C. Slater and K.H. Johnson, Phys. Rev. B5, 844 (1972).
9. J.C. Slater, Quantum Theory of Molecules and Solids, Vol. 4 (New York: McGraw-Hill Book Co., Inc., 1973).

electron. This approach allows the calculation of total energy differences by an approximation involving only single-electron orbital energies (eigenvalues); i.e.,

$$E_o(n_i) - E_e(n_{i-1}) \approx \epsilon_i(n_i - 1/2), \quad (11)$$

where E_o is the total electronic energy of a system having an initial electron in the i^{th} orbital. An electron is excited out of this i^{th} orbital into the continuum, and E_e is the total electronic energy of this final state. The single-electron eigenvalue, ϵ_i , which is calculated with the occupation of the i^{th} orbital halfway between that of the original and final states, is a good approximation to this total energy difference, especially for excitations involving valence electrons. (For core electrons another term 10 appearing on the right-hand side of Eq. (11) may be significant.) The advantage of this procedure is that single-electron orbital energies are generally more readily calculable, and therefore less costly, than total energy differences. For an optical transition one-half electron is transferred from the lower to the upper level. There is no problem in combining this concept with the NMT correction described above: the effect of the change in occupation numbers enters through the change in the density and therefore in the potential terms in Eq. (9). For an optical transition it is, of course, necessary to calculate the NMT correction to both levels involved.

III. RESULTS

The multiple scattering X- α parameters, internuclear separations, and alpha exchange parameters used in the calculations reported here are given in Table I. Touching spheres, whose radii were chosen to be proportional to their Slater atomic radii, were used for the atomic regions. The α values were taken from atomic calculations for the atomic regions, with an averaged value for the intersphere and outer sphere regions.

10. D.A. Ringers, "X α Calculation of Transition Energies in Multiply Ionized Atoms," USA Ballistic Research Laboratory Report BRL MR 2766, July 1977. (AD #A043091)

TABLE I. Computational Parameters.

Molecule	r_e	α_N	α_O	α_C	α_S	α_{IS}
NO	2.1758	.74725	.74118			.74422
CO	2.17		.74118	.75331		.74725
SN	2.8765	.74952			.72183	.73274
H ₂ CO	2.2825 r_{C-O} 2.1090 r_{C-H} < OCH 133.3°		.74118	.75331		.75006

In Tables II through V and Figures 1 through 4 we give the ionization energies as determined by Δ SCF and by transition state

TABLE II. CO Ionization Energies (eV).

Level	MT-Transition	Δ SCF ¹¹	NMT-Transition	Experiment ¹²
0 1s	551.1	550.8	539.8	542.1
c 1s	304.9	303.4	302.9	295.9
3 σ	32.7	36.3	35.5	38.3
4 σ	19.1	20.5	19.4	20.1
1 π	18.1	17.1	16.3	17.2
5 σ	12.9	14.7	13.9	14.5

11. D.A. Ringers and J.B. Danese, "Quantum Chemistry, Chemisorption, and Erosion. I. Properties of Diatomic Molecules", USA Ballistic Research Laboratory Report BRL R 2023, October 1977. (AD #A050249)
12. K. Siegbahn, C. Nordling, G. Johansson, J. Hedman, P.F. Heden, K. Hamrin, U. Gelius, T. Bergmark, L.O. Werme, R. Manne, and Y. Baer, ESCA Applied to Free Molecules (Amsterdam: North-Holland Publishing Co., 1971).

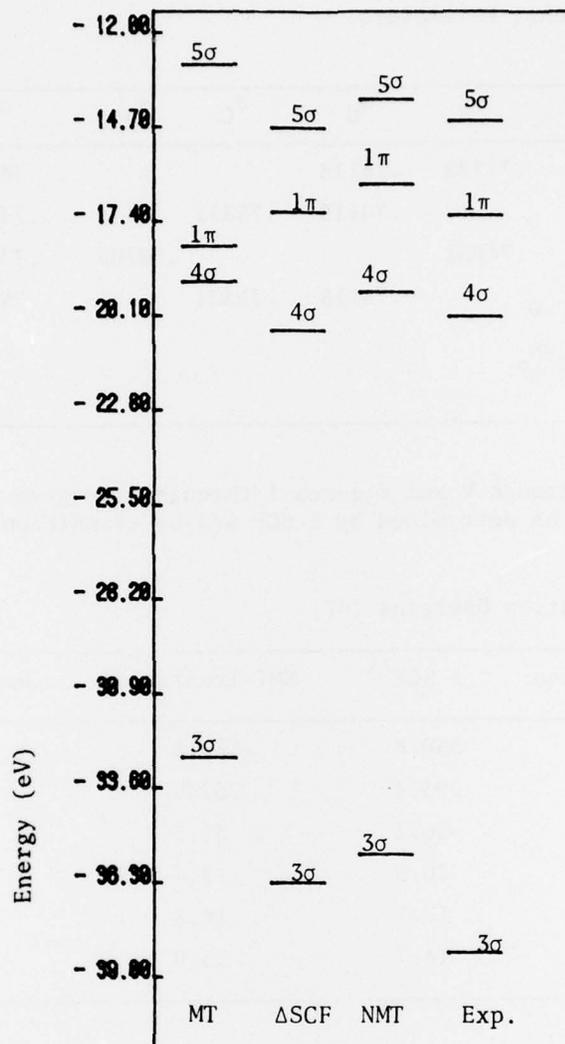


Figure 1. Ionization energies for CO.

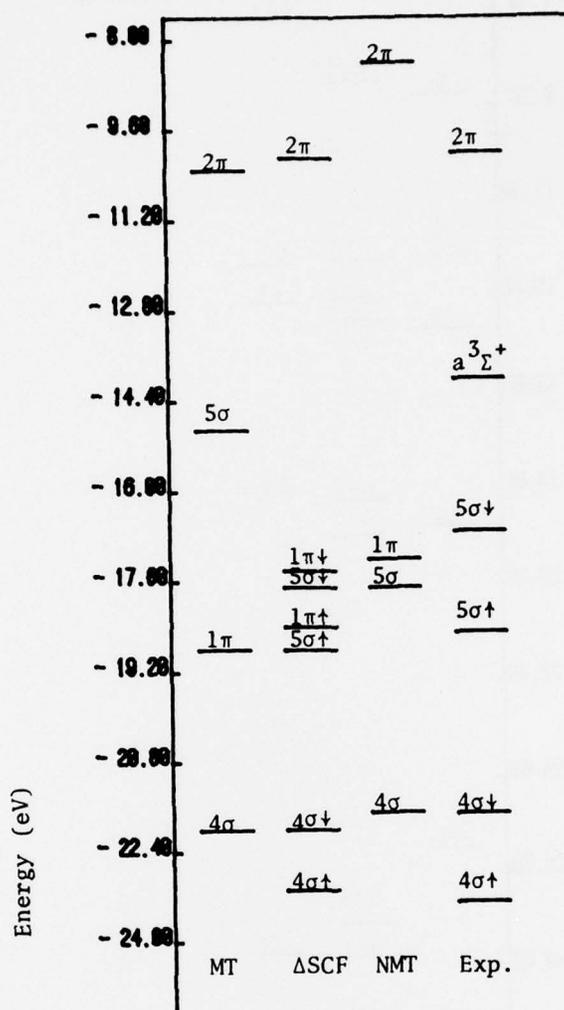


Figure 2. Ionization energies for NO.

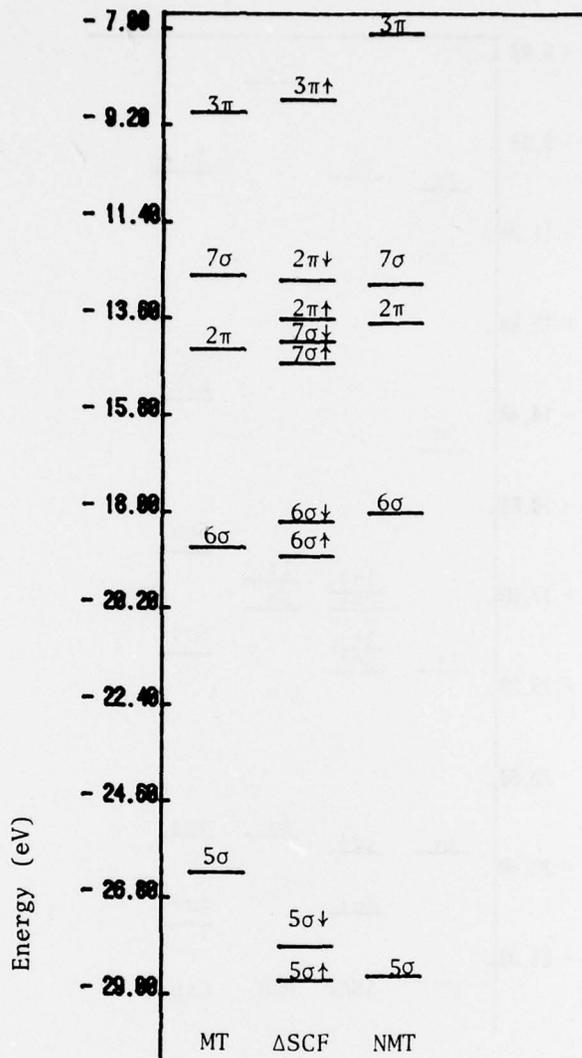


Figure 3. Ionization energies for SN.

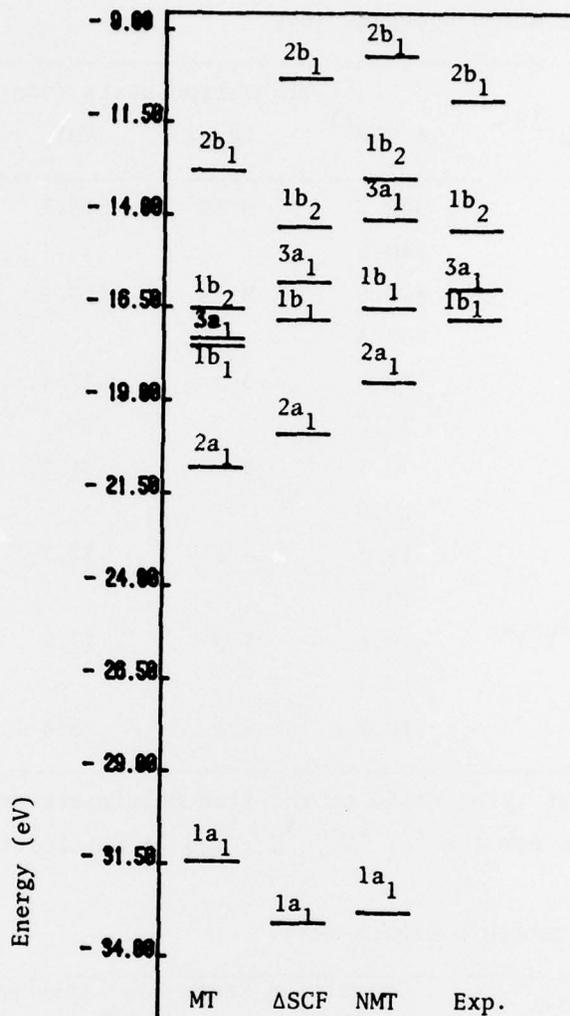


Figure 4. Ionization energies for HC OH.

TABLE III. NO Ionization Energies (eV).

Level	Experiment ¹²	Δ SCF ¹¹	Transition state (non-spin-polarized)		
			Level	NMT	MT
0 1s \uparrow	544.0	540.7	0 1s	543.7	551.6
0 1s \downarrow	543.3	540.5			
N 1s \uparrow	411.8	409.6	N 1s	415.2	419.3
N 1s \downarrow	410.3	408.3			
3 σ \uparrow	43.8	38.5	3 σ	37.4	34.4
3 σ \downarrow	40.6	37.7			
4 σ \uparrow	23.3	23.1	4 σ	21.7	22.0
4 σ \downarrow	21.7	22.0			
5 σ \uparrow	18.5	18.8	5 σ	17.7	14.9
5 σ \downarrow	16.7	17.7			
1 π \uparrow	14(a ³ Σ^+) ^a	18.4	1 π	17.2	18.8
1 π \downarrow		17.4			
2 π \uparrow	10	10.1	2 π	8.4	10.3

^aThis is the highest lying state of the five multiplets arising from the 1 π orbital. Values for the ¹ Δ , ¹ Σ^- , ³ Σ^- , and ³ Δ multiplets are not given.

TABLE IV. SN Ionization Energies (eV).

Level	Δ SCF ¹¹	Transition state (non-spin-polarized)		
		Level	NMT	MT
5 σ \uparrow	28.7	5 σ	28.6	26.2
5 σ \downarrow	27.9			
6 σ \uparrow	19.0	6 σ	18.0	18.8
6 σ \downarrow	18.2			
7 σ \uparrow	14.6	7 σ	13.7	12.6
7 σ \downarrow	14.1			
2 π \uparrow	13.6	2 π	12.8	14.3
2 π \downarrow	12.7			
3 π \uparrow	8.6	3 π	7.1	8.9

TABLE V. H₂CO Ionization Energies (eV).

Level	Experiment ¹³	Δ SCF	Transition state	
			NMT	MT
0 1s	542.1	546.3	529.3	547.9
C 1s		300.3	296.7	305.4
1 a ₁		33.1	32.8	31.4
1 b ₁	16.8	16.8	16.5	17.5
1 b ₂	14.4	14.3	13.0	16.5
2 a ₁		19.9	18.5	20.8
3 a ₁	16.0	15.8	14.1	17.3
2 b ₁	10.9	10.3	9.7	12.8

calculations for the molecules CO, NO, SN, and H₂CO. In each case all valence levels are reported for those orbitals which are occupied in the ground state. Except for SN, the core levels are reported as well. The levels denoted by arrows (\uparrow or \downarrow) were calculated in a spin-polarized manner using different orbitals for different spins. The Tables also list the MT-transition-state results so as to show the improvement obtainable with the NMT procedure. Tables VI and VII list the detailed contributions to the corrections for the CO molecule.

TABLE VI. NMT Contributions to Ionization Energies in CO (eV).

Level	$-\Delta E_L$	ΔE_Q	$-\Delta E_T$ (NMT)
0 1s	35.0	5.3	29.7
C 1s	34.6	3.7	30.9
3 σ	29.3	3.4	25.9
4 σ	32.4	4.1	28.3
1 π	34.1	3.7	30.4
5 σ	32.6	4.6	28.0

13. D. Turner, C. Baker, A.D. Baker, and C. Brandle, *Molecular Photoelectron Spectroscopy*, (New York: Wiley Interscience, 1970).

TABLE VII. NMT Contributions to Transition State Ionization Energies in CO (eV).

Level	$-\epsilon_i$ (MT)	$\Delta\epsilon_i$ (L)	$-\epsilon_i$ (NMT)	$-\epsilon_i$ (Experiment) ¹²
0 1s	551.1	11.0	540.0	542.1
C 1s	304.9	2.1	302.8	295.9
3 σ	32.7	- 2.8	35.5	38.3
4 σ	19.1	- 0.3	19.4	20.1
1 π	18.1	1.8	16.3	17.2
5 σ	12.9	- 1.0	13.9	14.5

Examination of the results shows the improvement achieved with the NMT linear correction and the agreement with experiment in the ionization energies.

One of the purposes of this study was to determine the importance of the quadratic density correction of Eq. (9), which may be related by the transition-state concept to a difference of quadratic corrections to the total energy. Examining Table VI, we see that the quadratic term for the total energy correction has an average value of 4.1 eV with the largest deviation for a valence state being 0.7 eV from this average value. Hence, if we use an average value, we make at most an error of 0.7 eV. Table VII also gives the directly calculated linear correction to the eigenvalues taken from Eq. (9). For the total energy differences it will, in many cases, not be necessary to calculate the quadratic term explicitly for each total energy state, or even for any total energy state, since the near equality of this term for most total energy states involved in ionization will cause large amounts of cancellation. For the calculation of excitations by the transition-state concept, the quadratic correction to the single-electron energy levels will in general not be necessary, since the near equality of the results with only the linear correction to the results obtained from a total difference calculation implies that there must be considerable cancellation among the quadratic corrections for single-electron eigenvalues as well as for total energy differences. The linear correction alone gives substantial improvement over the MT eigenvalues, as may be seen in the Tables and Figure 1. We conclude, then, that for the identification of ionization levels the quadratic term is necessary only for levels which are very close together. An example of just how close together the levels may be can be seen in the cases of SN and NO. The result using only the linear correction term gives the correct ordering for the levels which are found to be

separated by only .025 rydberg in the more complete calculation (one including quadratic terms) and in fact differs from the more complete calculation by only .006 rydberg.

The linear-correction result compares favorably with the discrete variational method (DVM)⁵, Felton-Sambe⁶, Hartree-Foch¹⁴ using Koopman's theorem, and overlapping sphere⁴ results for NO. For SN, however, the overlapping sphere results give an inverted ordering which has the 7σ level appearing above the 2π level. The ordering of the SN and NO ionization levels was found to be independent of whether the calculations were done spin-polarized or non-spin-polarized and whether the energy differences were calculated as differences in total energies or were approximated by the transition state technique.

The core levels of CO compare favorably with experiment but not so well as the valence levels. Further study is required to determine whether the core levels might not be improved or whether systematics exist in the behavior of these levels in similar systems.

IV. CONCLUSIONS

The inclusion of NMT corrections to the $X\alpha$ procedure generally used to calculate electronic energy levels has significantly increased the accuracy of the calculated values. When combined with the transition state method, the procedure is a viable one for the calculation of approximate total energy differences such as excitation energies.

It has been previously shown that the quadratic correction term in the expression for the total energy, while the most time consuming to calculate, is in general small and may usually be neglected when calculating total energy differences. The excitation and ionization energies calculated using the linear correction to single electron eigenvalues (by the transition state method) agree well with the values obtained from total energy differences. This implies that the quadratic correction for single-electron eigenvalues must likewise be small and may often be regarded as negligible.

The calculated excitation energies are somewhat less accurate than those determined from $X\alpha$ non-muffin-tin total energy differences. The determination of an excitation energy by total energy differences, however, requires two quite accurate calculations; one for the initial state and one for the final state. Thus the slight decrease in accuracy in the present method is offset by the need for only one calculation when using this procedure for calculating excitation energies.

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