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NONTRANSFERABLE CORRELATION EFFECTS AND MULTIPLET OSCILLATOR STRENGTHS FOR ELECTRIC DIPOLE TRANSITIONS IN ATOMS WITH RESULTS ON C II, N I, N II, N III, O II, O III, O IV, F II, AND Ne II

PAUL WESTHAUS
Department of Physics, Oklahoma State University, Stillwater
AND
OKTAY SINANOĞLU
Department of Chemistry, Yale University
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ABSTRACT

Wave functions which include selected, state-dependent correlation effects are used to evaluate multiplet oscillator strengths for a number of $1s^22s^22p^n \rightarrow 1s^22s2p^{n+1}$ electric dipole transitions in the first-row atoms and ions. It has long been known that those transitions cannot be accurately calculated within the Restricted Hartree-Fock approximation. Our results show that the usual improvement on this scheme, the mixing of those few configurations nearly degenerate with the Restricted Hartree-Fock (RHF) configuration, is by itself incapable of bringing the oscillator strengths into agreement with experimental values. Additional correlation effects which show up in the open-shell many-electron theory of atomic structure (MET) developed recently by Sinanoğlu and co-workers need also be considered. Calculations including all these highly state-dependent correlation effects yield very good agreement with available experimental values. These calculated oscillator strengths, together with many more for which experimental results are not available, are tabulated.

I. INTRODUCTION

In this article we present calculations of multiplet absorption oscillator strengths for electric dipole transitions in some atomic species of the first-row elements using a theory developed recently by Sinanoğlu and co-workers to include correlation effects.

The two expressions (Weiss 1967),

$$f_R(\gamma LS \rightarrow \gamma' L'S') = \tfrac{2}{3}\frac{E(\gamma' L'S') - E(\gamma LS)}{(2L+1)(2S+1)} \times \sum_{M_L=-L}^{L}\sum_{M_S=-S}^{S}\sum_{M_{L'}=-L'}^{L'}\sum_{M_{S'}=-S'}^{S'} |\langle \Psi_{\gamma LSM_LM_S} | \boldsymbol{R} | \Psi_{\gamma' L'S'M_{L'}M_{S'}} \rangle|^2 \quad (1)$$

in terms of the dipole-length operator,

$$\boldsymbol{R} = \sum_{i=1}^{N} \boldsymbol{r}_i ,$$

and

$$f_\nabla(\gamma LS \rightarrow \gamma' L'S') = \tfrac{2}{3}\frac{1}{(2L+1)(2S+1)\{E(\gamma' L'S') - E(\gamma LS)\}} \times \sum_{M_L=-L}^{L}\sum_{M_S=-S}^{S}\sum_{M_{L'}=-L'}^{L'}\sum_{M_{S'}=-S'}^{S'} |\langle \Psi_{\gamma LSM_LM_S} | \boldsymbol{\nabla} | \Psi_{\gamma' L'S'M_{L'}M_{S'}} \rangle|^2 \quad (2)$$

in terms of the dipole-velocity operator,

$$\boldsymbol{\nabla} = \sum_{i=1}^{N} \boldsymbol{\nabla}_i ,$$

give identical numerical results when the Ψ's and E's are the exact eigenfunctions and eigenvalues of the nonrelativistic Hamiltonian,

$$H = -\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N}\frac{-Z}{|r_i|} + \sum_{i<j}\frac{1}{|r_i - r_j|}\,. \tag{3}$$

(Atomic units ($\hbar = 1$, $m_e = 1$, $Q_e = 1$) are used throughout.) In equations (1) and (2) the angular-bracket notation indicates the matrix elements of an operator $\mathcal{O}$,

$$\langle \Psi_{\gamma LSM_L M_S} | \mathcal{O} | \Psi_{\gamma' L'S'M_{L'}M_{S'}} \rangle$$

$$= \frac{\int dx_1 \ldots dx_N \Psi^{*(x_1 \ldots x_N)}_{\gamma LSM_L M_S} \mathcal{O}(1 \ldots N) \Psi^{(x_1 \ldots x_N)}_{\gamma' L'S'M_{L'}M_{S'}}}{[(\int dx_1 \ldots dx_N |\Psi^{(x_1 \ldots x_N)}_{\gamma LSM_L M_S}|^2)(\int dx_1 \ldots dx_N |\Psi^{(x_1 \ldots x_N)}_{\gamma' L'S'M_{L'}M_{S'}}|^2)]^{1/2}}\,.$$

In the standard notation, L, S, and M_L, M_S are the quantum numbers associated with the total orbital angular momentum, total spin, and the Z-components of these quantities; γ stands for the orbital configuration of the state.

Most often, approximate independent-particle model wave functions are used to evaluate the transition matrix elements. The energies are then evaluated as the corresponding expectation values of H. Viewing the electric dipole transitions as one electron jumps between outer orbitals (and neglecting changes in the inner orbitals) leads to approximations for f_R and f_∇ involving only one-body integrals between the final and initial orbitals (Goldberg 1935; Bates and Damgaard 1949). When the $(N - 1)$ passive electrons form a closed-shell, self-consistent field, calculations of the initial and final orbitals of the jumping electron lead to accurate results for the oscillator strengths (Weiss 1963). In fact, even with these initial and final orbitals determined by cruder approaches such as the Coulomb approximation (Bates and Damgaard 1949), good, sometimes excellent, results are obtained for the oscillator strengths. However, for transitions involving equivalent electrons in open shells in either or both terms, the oscillator strengths obtained with Restricted Hartree-Fock (RHF) wave functions usually are in poor agreement with experiment, differing in many instances by a factor of 2 or 3 (Kelly 1964*a*, *b;* Pfennig, Steele, and Trefftz 1965). Electron correlation—either entirely or in some portion significant for determining oscillator strengths—needs to be taken into account in such cases.

For computations of oscillator strengths involving equivalent electrons, Layzer (1959) has indicated the need of mixing nearly degenerate configurations (complexes) with the RHF wave function. Froese (1965) has carried out this prescription in her "zero-order mixing" calculations on first-row atoms. A similar approach has been taken by Dalgarno and his collaborators (Cohen and Dalgarno 1964; Crossley and Dalgarno 1965). These calculations involve the mixing of but a few terms. In a somewhat opposite vein, Weiss (1967) has calculated correlated wave functions via large-scale configuration interaction (CI) in order to compute oscillator strengths for carbon and its ions.

The results of Froese and Dalgarno, although improving on the RHF approximation, are still not generally in agreement with experiment. Additional configurations, supplementing those degenerate with the RHF wave function, must also be included. On the other hand, the straightforward CI procedure followed by Weiss does not attempt to select a priori what are likely to be the significant configurations in the oscillator strength calculations. All configurations important for determining energy are (probably) not of equal importance in computing oscillator strengths which would seem to depend strongly only upon those configurations needed to specify an accurate charge distribution. Thus Weiss's approach may be very inefficient when one is interested in just oscillator strengths. A formalism in which the correlation effects significant in the computation of

oscillator strengths can be isolated and determined independently would be most advantageous.

II. THE "MANY-ELECTRON THEORY OF ATOMS AND MOLECULES" ("MET") APPROACH FOR INCLUSION OF CORRELATION EFFECTS

Over the past few years Sinanoğlu and his co-workers have developed a theory of electron correlation in atoms and molecules. Sinanoğlu has shown that the Hartree-Fock part of the wave function takes care of most of the long-range part of the Coulomb repulsion, and once this is taken out, the correlation effects result from the shorter-range "fluctuation potentials" between electrons (Sinanoğlu 1962). For closed-shell systems, the short range of this potential and the "exclusion" effects studied by perturbation theory (Sinanoğlu 1960, 1961) cause decoupled-pair correlations to become dominant. This approach was later generalized into a nonperturbative many-electron theory of atoms and molecules (MET) (Sinanoğlu 1962, 1964). Methods of examining the 1-, 3-, 4-, . . . electron correlations as well as the dominant pair correlations were developed. Thus the N-electron correlation problem was systematically reduced to $\frac{1}{2}N(N-1)$ separate two-electron problems and additional effects.

In nonclosed (open) shell states, other novel correlation effects arise. These were first studied in a perturbation approach for open shells developed by Silverstone and Sinanoğlu (1966). Later the theory was generalized into a nonperturbative approach (Sinanoğlu 1968) and applied by Sinanoğlu and Öksüz to atomic-structure calculations (Sinanoğlu and Öksüz 1968; Öksüz and Sinanoğlu 1969). A mathematical analysis of the open-shell wave function resulting in the nonperturbative theory will be presented by Westhaus and Sinanoğlu (1969). The RHF wave function is the starting point of this formalism. Then, according to the nonperturbative treatment, correlations among electrons occupying the RHF orbitals separate mathematically and physically into three types:

Type I. *Internal correlations* consist of virtual excitations of electrons from occupied to vacant orbitals in the Hartree-Fock sea. These are schematically depicted in Figure 1. The main part of this effect occurs in near-degeneracy CI calculations or equivalently in multiconfigurational self-consistent field calculations.

Type II. *Semi-internal correlations* arise from virtual excitations in which at least one but not all excited electrons are expelled from the Hartree-Fock sea. The two-body correlations, in which one electron is expelled from the Hartree-Fock sea while the other is excited to a previously unoccupied orbital in the sea, first arose in the perturbative treatment and presumably dominate the remaining semi-internal effects. These are illustrated in Figure 2.

Type III. *All-external correlations* chiefly occur as excitations of decoupled electron pairs from the Hartree-Fock sea, but generally include correlation effects depicted by virtual expulsions of all excited electrons from the sea (see Fig. 3). Only the all-external correlations occur in the MET description of closed-shell states; the internal and semi-internal correlations are unique to open-shell states.

Consideration of all three types of correlations involving 1, 2, . . . , N particles leads to expressing the exact open-shell electronic wave function as

$$\Psi = \Phi_{\mathrm{RHF}} + \chi(\text{internal}) + \chi(\text{semi-internal}) + \chi(\text{all-external}) \; . \tag{4}$$

With the normalization

$$\int dx_1 \ldots dx_N \Phi^*_{\mathrm{RHF}}(x_1 \ldots x_N)\Psi(x_1 \ldots x_N) = \int dx_1 \ldots dx_N \Phi^*_{\mathrm{RHF}}(x_1 \ldots x_N)\Phi_{\mathrm{RHF}}(x_1 \ldots x_N) = 1 \; . \tag{5}$$

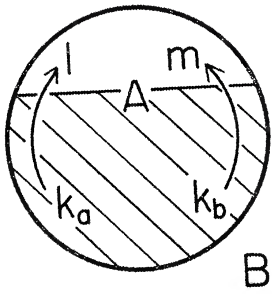

FIG. 1

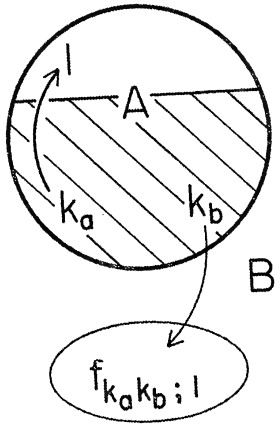

FIG. 2

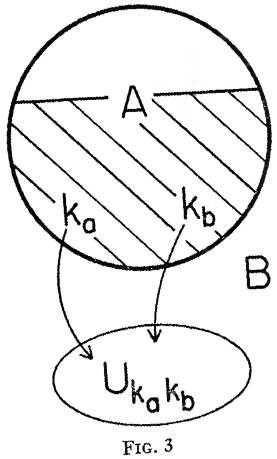

FIG. 3

FIG. 1.—*An internal correlation:* Electrons shift from occupied to unoccupied orbitals within the Hartree-Fock sea (A).

FIG. 2.—*A semi-internal correlation:* One electron shifts within the Hartree-Fock sea (A), while a second electron is expelled to the one-particle function $f_{k_a k_b; l}$ in B.

FIG. 3.—*An all-external pair correlation:* Both electrons are ejected from the Hartree-Fock sea (A) into a pair correlation function $U_{k_a k_b}$ in B similar to those occurring in closed shell MET.

With the M ($>N$) orbitals $\phi_1, \phi_2, \ldots, \phi_M$ comprising the Hartree-Fock sea, we can construct $\binom{M}{N}$ Slater determinants Δ_K and write Φ_{RHF} in terms of the first $\mathcal{K}$ members of this set of determinants,

$$\Phi_{\mathrm{RHF}}(x_1 \ldots x_N) = \sum_{K=1}^{\mathcal{K}} C_K \Delta_K = \sum_{K=1}^{\mathcal{K}} C_K \frac{\mathcal{A}(N)}{\sqrt{N!}} [\phi_{k_1}(x_1) \ldots \phi_{k_N}(x_N)] . \tag{6}$$

The index K represents an N-tuple of orbital labels $k_1, k_2, \ldots, k_N$, and $\mathcal{A}(N)$ is the N-particle antisymmetrizer. The correlations due to excitations from orbitals in determinants 1 through $\mathcal{K}$ to vacant orbitals within the Hartree-Fock sea can be depicted in terms of the remaining Slater determinants. Thus, χ(internal) can be expanded:

$$\chi(\text{internal}) = \Sigma d_K \Delta_K , \tag{7}$$

where the summation is extended over $K = \mathcal{K} + 1$ to $K = M!/N!(M - N)!$ The remaining part of the correlation wave function can be written

$$\chi(\text{semi-internal}) + \chi(\text{all-external}) = \sum_{K=1}^{\mathcal{K}} C_K \chi^K = \chi_f + \chi_U , \tag{8}$$

where the correlations in χ^K can be depicted in terms of semi-internal and all-external correlation functions (Silverstone and Sinanoğlu 1966), such as $f^K{}_{kikj;l}$ and $U^K{}_{kikj}$.

$$\begin{aligned}
\chi^K = \frac{\mathcal{A}(N)}{\sqrt{N!}} \Big\{ [\phi_{k_1}(x_1) \ldots \phi_{k_N}(x_N)] \Big[\sum_{i=1}^{N} \frac{f_{k_i}{}^K(x_i)}{\phi_{k_i}(x_i)} \\
+ \sum_{i<j}^{N} \sum_{l \notin K} \frac{f^K{}_{k_i k_j; l}(x_i)\phi_l(x_j)}{\phi_{k_i}(x_i)\phi_{k_j}(x_j)} + \ldots \Big] \Big\} \\
+ \frac{\mathcal{A}(N)}{\sqrt{N!}} \Big\{ [\phi_{k_1}(x_1) \ldots \phi_{k_N}(x_N)] \Big[\frac{1}{\sqrt{2}} \sum_{i<j}^{N} \frac{U^K{}_{k_i k_j}(x_i, x_j)}{\phi_{k_i}(x_i)\phi_{k_j}(x_j)} \\
+ \tfrac{1}{2} \sum_{\substack{i<j \\ \{i,j\} \neq \{l,m\}}} \sum_{l<m} \frac{U^K{}_{k_i k_j}(x_i, x_j)}{\phi_{k_i}(x_i)\phi_{k_j}(x_j)} \frac{U^K{}_{k_l k_m}(x_l, x_m)}{\phi_{k_l}(x_l)\phi_{k_m}(x_m)} + \ldots \Big] \Big\} \\
= \chi_f{}^K + \chi_U{}^K .
\end{aligned} \tag{9}$$

In writing equation (9) we have grouped the all-external single-particle correlations (orbital polarizations) with the semi-internal correlations in $\chi_f{}^K$, for not only are the former more closely related physically to the latter than to the remaining all-external correlations, but also both are amenable to the same mathematical techniques (Silverstone and Sinanoğlu 1966; Sinanoğlu 1968; Öksüz and Sinanoğlu 1969). With a fuller explanation of the correlation functions given in the references just cited, it suffices to say that the semi-internal correlation of two electrons occupying orbitals k_i and k_j in determinant K in Φ_{RHF} results in one being scattered to a vacant orbital l with the other electron described by $f^K{}_{kikj;l}$. The all-external correlation of two electrons occupying orbitals k_i and k_j in determinant K is depicted by the two-particle function $U^K{}_{kiki}$ (see Figs. 2 and 3). The correlations depicted by χ(internal) and χ(semi-internal), together with the single-particle excitations (polarizations) in χ(all-external), i.e.,

$$\chi(\text{internal}) + \sum_{K=1}^{\mathcal{K}} C_K \chi_f{}^K ,$$

are called nondynamical and are highly specific to the state under consideration (i.e., they are nontransferable). The remaining correlations, termed dynamical, can most probably be transferred.

The nondynamical correlations, unlike the dynamical ones, can be analyzed by a limited CI, with the configurations to be mixed clearly indicated by MET (Silverstone and Sinanoğlu 1966; Sinanoğlu and Öksüz 1968; Öksüz and Sinanoğlu 1969).

Charge distributions for open-shell states should be accurately portrayed in terms of the RHF orbitals and the *nondynamical correlations*. This conjecture is based partly on analogy to the closed-shell case, where the dynamical correlations (two-body excitations and unlinked cluster products, in the MET sense [Sinanoğlu 1964], of two-body correlations) have negligible effect upon the Hartree-Fock charge distribution. Thus we expect that accurate oscillator strengths may be computed even when only the nondynamical correlation effects are included in the wave function.

The calculations of Froese (1965) and of Cohen and Dalgarno (1964) take into account only what we have termed internal correlation. We have used the open-shell wave functions containing *all the nondynamical correlations*, including the new "semi-internal" effect, obtained by Sinanoğlu and Öksüz to compute the electric dipole oscillator strengths. These MET wave functions have been obtained using a fully automatic program for 113 states of the $1s^2 2s^m 2p^n (m = 0,1,2; 0 \leq n \leq 6)$ configurations in the atoms B through Na and their ions. These wave functions are among the most detailed available at present and have formed the basis for Sinanoğlu and Öksüz's theory of atomic structure (Sinanoğlu and Öksüz 1968; Ösküz and Sinanoğlu 1969).

III. DISCUSSION OF RESULTS

The absorption oscillator strengths for twenty-eight ultraviolet transitions in the first-row atoms and ions are listed in Table 1. Our calculations were carried out according to four different schemes with the option of using (*a*) the Restricted Hartree-Fock (RHF) or the many-electron theory (MET) wave functions (Sinanoğlu and Öksüz 1968; Öksüz and Sinanoğlu 1969); (*b*) formulae based on the dipole-length operator $\boldsymbol{R}$ or the dipole-velocity operator $\boldsymbol{\nabla}$. Columns (2) and (3) contain the results of our RHF calculations using $\boldsymbol{R}$ and $\boldsymbol{\nabla}$, respectively. A similar arrangement is found in columns (5) and (6), where the results are obtained with the MET wave functions. Separating these two sets of calculations are the currently (1966) accepted values of the oscillator strengths as listed in the National Bureau of Standards (NBS) tables (Wiese, Smith, and Glennon 1966). The final column contains the available experimental data. In all our calculations the energies were computed as the expectation value of the Hamiltonian with respect to the corresponding wave function.

The influence of the nondynamical correlations is felt substantially in virtually all the cases considered. Changes in the computed oscillator strengths by factors of 2–3 due to correlation effects are not uncommon. With but few exceptions we find $f_R^{\mathrm{RHF}} > f_R^{\mathrm{MET}}$, i.e., the RHF calculations usually, but not always, overestimate f_R. The exceptions point out the highly specific character of the effects introduced by the nondynamical-type correlations. In addition, our results underscore the fact that agreement between f_R and f_∇ obtained with RHF wave functions does not insure their accuracy (La Paglia 1967*a*, *b*). In more than one case we find that, although $f_R^{\mathrm{RHF}} \approx f_\nabla^{\mathrm{RHF}}$, these values are drastically changed upon introducing the nondynamical-type correlations. The $^2P \rightarrow {}^2D$ multiplet in C II is a clear illustration of this point. There are, of course, many more instances in which f_R^{RHF} and f_∇^{RHF} do *not* agree, as exemplified in the $^2P \rightarrow {}^2P$ transitions in C II. Often they differ by a factor of 2–3. On the other hand, the agreement between f_R^{MET} and f_∇^{MET} is *consistently* good, usually within 15 percent.

Of particular significance is the very good agreement obtained between the available experimental data (Labuhn 1965; Hinnov 1966; Lawrence and Savage 1966; Heroux 1967; Bickel 1967) and the corresponding MET values, especially in light of the sub-

stantial changes which must be introduced into the RHF results. In the present compilation it is interesting to note that in two instances (Labuhn 1965; Lawrence and Savage 1966; Hinnov 1966) there is a discrepancy between two sets of experimental data. In both cases the MET results clearly favor one experiment over the other.[1] The MET results may be useful in evaluating experimental data when similar conflicts arise. Certainly the agreement with the other experimental values is encouraging in this respect. In addition, we feel confident about using the MET values in that majority of cases where

TABLE 1

MULTIPLET ABSORPTION OSCILLATOR STRENGTHS

Transition (1)		f_R^{RHF} (2)	f_V^{RHF} (3)	f^{NBS} (4)	f_R^{MET} (5)	f_V^{MET} (6)	f^{Exp} (7)
C II	$2p\ ^2P \rightarrow 2p^2\ ^2D$	0 263	0.262	0.27	0.125	0.134	0 114[a]
N III	$2p\ ^2P \rightarrow 2p^2\ ^2D$	.213	.214	.18	.114	.125	0 103[b]
O IV	$2p\ ^2P \rightarrow 2p^2\ ^2D$	.179	.181	.15	.106	.111	0.091[c]
C II	$2p\ ^2P \rightarrow 2p^2\ ^2S$	.070	.042	.059	.122	.121	
N III	$2p\ ^2P \rightarrow 2p^2\ ^2S$	.056	.035	.11	085	.084	
O IV	$2p\ ^2P \rightarrow 2p^2\ ^2S$	047	.030	.10	.069	.071	
C II	$2p\ ^2P \rightarrow 2p^2\ ^2P$	.736	.282	.52	.501	.471	
N III	$2p\ ^2P \rightarrow 2p^2\ ^2P$	.577	227	.45	.399	.390	0.416[b]
O IV	$2p\ ^2P \rightarrow 2p^2\ ^2P$	473	.189	.38	334	.329	
N II	$2p^2\ ^3P \rightarrow 2p^3\ ^3D$	.236	268	.17	.100	.105	0 109[a],0 101[b]
O III	$2p^2\ ^3P \rightarrow 2p^3\ ^3D$	.200	.225	.15	.100	.104	0 102[c]
N II	$2p^2\ ^3P \rightarrow 2p^3\ ^3P$	.170	.138	.22	.137	.155	0 131[b]
O III	$2p^2\ ^3P \rightarrow 2p^3\ ^3P$	.143	.117	.18	127	.135	
N II	$2p^2\ ^3P \rightarrow 2p^3\ ^3S$	.334	.110	.23	218	.203	0 189[b]
O III	$2p^2\ ^3P \rightarrow 2p^3\ ^3S$	.272	.092	.19	.183	.173	
N II	$2p^2\ ^1D \rightarrow 2p^3\ ^1D$	.651	.310	.45	.314	.327	
O III	$2p^2\ ^1D \rightarrow 2p^3\ ^1D$	.534	.263	.37	.297	303	
N II	$2p^2\ ^1D \rightarrow 2p^3\ ^1P$	.245	.094	.30	.298	.261	
O III	$2p^2\ ^1D \rightarrow 2p^3\ ^1P$	.202	.080	.25	.219	193	
N II	$2p^2\ ^1S \rightarrow 2p^3\ ^1P$	.817	.457	.40	.259	.309	
O III	$2p^2\ ^1S \rightarrow 2p^3\ ^1P$	.669	.338	.35	.294	.337	
N I	$2p^3\ ^4S \rightarrow 2p^4\ ^4P$	.503	.542	.13	.145	176	0.080[a],0 13[d]
O II	$2p^3\ ^4S \rightarrow 2p^4\ ^4P$	.428	.457	.43	.206	.225	0 182
O II	$2p^3\ ^2D \rightarrow 2p^4\ ^2D$	.263	.189	.25	.141	.167	
O II	$2p^3\ ^2P \rightarrow 2p^4\ ^2S$	.125	081	.15	097	.102	
O II	$2p^3\ ^2P \rightarrow 2p^4\ ^2D$	.126	.122	.07	.030	.043	
F II	$2p^4\ ^3P \rightarrow 2p^5\ ^3P$	.322	263	.56	.140	.172	
Ne II	$2p^5\ ^2P \rightarrow 2p^6\ ^2S$	0 176	0 117	0 33	0 073	0.091	0 035[e],>0 055[f]

NOTE.—The notation is explained in text.

REFERENCES.—(*a*) Lawrence and Savage (1966); (*b*) Heroux (1967); (*c*) Bickel (1967); (*d*) Labuhn (1965); (*e*) Hinnov (1966); (*f*) unpublished work of G. M. Lawrence and J. Hesser.

no experimental corroboration yet exists. Thus we hope our MET values may be of immediate use in astrophysical applications.

On the basis of comparison with available experimental results, the MET values are generally quite superior to those tabulated in the NBS Tables, although the latter often represent a substantial improvement upon the RHF results by including limited CI in the form of the "double configuration" approximation (Bolotin and Yutsis 1953; Bolotin, Levison and Levin 1956; Steele and Trefftz 1966). As we pointed our earlier, these limited CI calculations aim at including part of what MET refers to as internal-type correlation. Apparently, such limited CI is not always sufficient to bring the calculated

[1] Lawrence (private communication) has remeasured the $4S \rightarrow 4P$ oscillator strength for N I and finds it in substantial agreement with his earlier result, which is approximately one-half the MET value reported here.

oscillator strengths into agreement with experiments—the remaining nondynamical-type correlations are also important. To illustrate this, we present in Table 2 the results of four types of calculations on eight representative transitions: Column (2) lists our f_R^{RHF}, our Restricted Hartree-Fock results. Successive columns list results obtained after the introduction of one or more specific types of nondynamical correlations: f_R^{CD} denotes the results of Cohen and Dalgarno (1964), who introduce internal correlation into the lower states by mixing configurations degenerate with the RHF wave function (χ(internal) $\equiv 0$ for the upper states of transitions listed in Table 2). The notation f_R^{INL} denotes another of our calculations in which, while internal correlations alone were introduced into the lower states, the upper states contained all possible nondynamical correlations. Column (5) tabulates f_R^{MET} containing all nondynamical correlations in both terms, while the experimental values are displayed in the last column. Comparing f_R^{RHF} and f_R^{CD}, we conclude that the internal correlations in the ground state do play a major role. With but one exception, the results of Cohen and Dalgarno do correct the

TABLE 2

COMPARISON OF MULTIPLET ABSORPTION OSCILLATOR STRENGTHS FOR TRANSITIONS BETWEEN STATES IN WHICH VARIOUS PARTS OF NONDYNAMICAL CORRELATION EFFECTS ARE INCLUDED

Transition (1)		f_R^{RHF} (2)	f_R^{CD} (3)	f_R^{INL} (4)	f_R^{MET} (5)	f^{Exp} (6)
C II	$^2P \rightarrow {}^2D$	0 263	0 204	0 121	0 125	0 114[a]
N II	$^3P \rightarrow {}^3D$	.236	.192	097	100	.109[a] / 101[b]
N II	$^3P \rightarrow {}^3P$	170	213	.175	.137	.131[b]
N II	$^3P \rightarrow {}^3S$	.334	.244	.226	218	.189[b]
N III	$^2P \rightarrow {}^2D$	.213	167	114	114	103[b]
N III	$^2P \rightarrow {}^2P$	.577	.415	.404	399	.416[b]
O III	$^3P \rightarrow {}^3D$	200	.162	097	100	102[c]
O IV	$^2P \rightarrow {}^2D$	0.179	0 141	0 105	0 106	0.091[c]

NOTE.—The notation is explained in the text.

REFERENCES.—(*a*) Lawrence and Savage (1966); (*b*) Heroux (1967); (*c*) Bickel (1967).

RHF values in the right directions. Furthermore, when the semi-internal and polarization corrections are introduced only into the upper state—that is, when internal effects alone are considered in the lower state—agreement with the full MET calculations is often very good. Note, however, that when the internal correlations are suppressed by symmetry as they are in the upper state, the remaining nondynamical type correlations *must* be included to obtain the reasonable agreement with experiment (compare f_R^{CD} and f_R^{INL} with f_R^{MET} and experiment). Thus, the significant role played here by the internal correlations in the lower state does not diminish the importance of including other nondynamical effects in the calculations. The internal correlations are highly specific to transitions from the ground state. Indeed, in transitions from higher states, internal correlations (i.e., hole-pair excitations [La Paglia and Sinanoğlu 1966]) may be absent, in which case the remaining nondynamical effects assume the entire burden of modifying the RHF results. Thus we conclude that *all* nondynamical-type correlation as analyzed within the framework of MET should be included in the wave functions to obtain accurate oscillator strengths.

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