PHYSICAL REVIEW A

GENERAL PHYSICS

THIRD SERIES, VOLUME 28, NUMBER 6 DECEMBER 1983

Multiconfiguration Hartree-Fock results with Breit-Pauli corrections for forbidden transitions in the $2p^4$ configuration

Charlotte Froese Fischer and H. P. Saha
Box 6035B, Vanderbilt University, Nashville, Tennessee 37235

(Received 15 July 1983)

Energy levels and fine-structure splittings are calculated for the ground-state configuration of the oxygen isoelectronic sequence using the multiconfiguration Hartree-Fock method with Breit-Pauli corrections. Electric quadrupole and magnetic dipole transition probabilities are reported for transitions between several of these levels. Our results are compared with those from other theories and, in the case of energy levels, also with observation. For degrees of ionization up to about 12 ($Z=20$), our energy levels are in better agreement with observation than other theories, but for ${}^1D_2$ a relatively larger, systematic discrepancy remains.

I. INTRODUCTION

Energy levels and transition probabilities are fundamental atomic properties of importance in both astrophysics[1] and fusion research.[2] By comparing the difference between theoretical multiconfiguration Dirac-Hartree-Fock[3] (MCDHF) results and observation of levels in the $n=2$ complex, Edlén[4] has been able to predict accurate transition energies, not only for lines already observed, but also for unobserved or possibly unidentified lines of highly ionized systems. Systematic differences were found between theory and observation particularly at lower stages of ionization, indicating that theory had not accounted for all effects. Transition probabilities are not known nearly as reliably as transition energies and few experimental results are available. Of particular interest are the forbidden transition probabilities necessary for the interpretation of forbidden line intensities which may provide valuable astrophysical information. The MCDHF results of Cheng *et al.*[3] referred to earlier, included only a limited amount of correlation which, for low degrees of ionization, is known to be inadequate for the accurate determination of atomic properties. The multiconfiguration Hartree-Fock method with the Breit-Pauli correction (MCHF + BP) differs in that it is not expected to be as reliable for highly ionized systems, but can include correlation more readily. Thus, in a sense, it complements MCDHF.

In this work, we calculated the energy levels and forbidden transition probabilities between the fine structure levels of the $2p^4$ ground configuration of neutral oxygen and many ions of isoelectronic sequence. Two wave-function expansions were used. In the first, the expansions included only configurations in the $n=2$ complex, which is the MCHF + BP equivalent of the MCDHF approach used by Cheng *et al.* In the second, many configurations outside the complex were also included. Thus, a comparison of these two results would indicate the importance of correlation outside the complex whereas a comparison of the former with MCDHF, particularly at high Z, would identify the pure relativistic effects that cannot be accounted for in the Breit-Pauli approximation.

A few forbidden transition probabilities for the ground configurations of the oxygen isoelectronic sequence have been reported by Kastner *et al.*[5] using the SUPERSTRUCTURE program developed at University College of London. They allow for configuration interaction between a limited number of configurations and also include relativistic corrections as described by Eissner *et al.*[6] However, no systematic study of the reliability of their results was reported.

II. COMPUTATIONAL PROCEDURE

The MCHF + BP method determines a wave function in two stages. In the first stage, a variational calculation is performed for orbitals of a particular L,S state using the MCHF method.[7] In the present calculation, the ${}^3P$ state was selected, though results were not sensitive to this choice. Then, with these orbitals fixed, in the second stage the Breit-Pauli interaction matrix is determined for a large set of configuration states, including a number of different L,S states. The eigenvalues and eigenvectors of this interaction matrix determine the total energy and wave-function expansion, respectively, of the L,S,J state.

We performed two sets of calculations—one where the configurations were restricted to the $n=2$ complex, the other was a more elaborate calculation with a lengthy expansion.

In the first case (which we refer to as the complex calculation), the radial functions were determined from a Hartree-Fock calculation for $2p^4\,{}^3P$ and the Breit-Pauli interaction matrix was over the set of the four configuration states of the $n=2$ complex, namely,

$$2s^22p^4\ {}^3P,{}^1D,{}^1S;2p^6\,{}^1S\ .$$

In the second calculation (which we shall refer to as the correlation calculation) we included a large number of configurations so that theoretical term energies would be in reasonable agreement with observation. In this case the variational MCHF calculation was over the set of 28 configuration states of the ${}^3P$ term, namely,

$$\{2s^22p^4,\ 2s\,3s\,({}^3S)2p^4,\ 2s^22p^3({}^2P,{}^4S)3p,\ 2s\,2p^4({}^2P,{}^4P,{}^2D)3d,\ 2s^22p^2({}^3P,{}^1D)3d^2,\ 2p^43d^2,\ 3s^22p^4,\ 2p^43p^2,\ 2p^53p\ ,$$
$$2s^22p^2({}^3P,{}^1D,{}^1S)3p^2,\ 2s\,3s\,({}^1S,{}^3S)2p^3({}^2P,{}^2D,{}^4D,{}^4S)3p,\ 2s^22p^3({}^4S)4p,\ 2p^54p,\ 2s\,2p^4({}^4P)4s\}\,{}^3P\ .$$

The inner $1s,2s,2p$ radial functions were kept fixed at their Hartree-Fock value. The above expansion was selected after a series of tests had been performed and represents the set of configurations whose mixing coefficients were greater than 0.01 in the case of oxygen.

The Breit-Pauli interaction matrix was over a set of 90 configuration states for the atomic number Z in the range 8—19 and 125 states for Z in the range 20—42. The 90 configuration states were selected from the following set of configurations with mixing coefficients greater than 0.006:

$$\{\,2s^22p^4,\ 2p^6,\ 2s\,2p^43d,\ 2s^22p^23p^2,\ 2s\,3s\,2p^33p,\ 2s^22p^33p,\ 2s^22p^23d^2,\ 2p^43d^2,\ 2s^22p^34p,\ 2s\,3s\,2p^4,\ 3s^22p^4,\ 2p^53p\ ,$$
$$2p^43p^2,\ 2p^54p,\ 2s^23s^22p^2,\ 2s\,2p^33p\,3d,\ 2s^23s\,2p^23d,\ 2s\,2p^44s\,\}({}^3P,{}^1D,{}^1S)\ .$$

A previous study of the MCHF + BP method applied to the boron sequence[8] suggested that for highly ionized systems the singly substituted states coupled to the reference configuration through the one-electron Pauli corrections became more important at high Z. For Z in the range 20—42 we included the following configurations in addition to the above, namely,

$$\{2s^22p^33p,\ 2s^22p^34p\}({}^3D,{}^5D,{}^3S)$$

and

$$\{3s\,2p^44s,\ 2s^22p^23p\,4p\}({}^3P,{}^1D,{}^1S)\ .$$

III. RESULTS AND DISCUSSION

A. Term energies

In Table I are reported the excitation energies (in cm^{-1}) from the $2s^22p^4\,{}^3P_2$ ground state of oxygenlike ions of all $2s^22p^4$ levels. Toward the low-Z end of the isoelectronic sequence, the most important correction to the complex (or the Hartree-Fock approximation) arises from the effect of correlation. The latter directly affects the term energy separation. As a check on the accuracy to which correlation has been accounted for in the wave-function expansion, we compare in Table II, the nonrelativistic ${}^1D$ and ${}^1S$ term energies relative to ${}^3P$ in oxygen with other theoretical results and observation. (The latter were obtained as a weighted average of observed levels.) MCDHF results are not available for oxygen but some term energies reported by Zeippen *et al.*[9] have been included. These are based on the scaled Thomas-Fermi-Dirac potential for deriving one-electron orbitals and a wave-function expansion of only ten configurations. In order to be able to compare MCHF + BP with this approximation, a special calculation was performed for this case which included the same configurations, the number being $m=10$. The third set of results in Table II for which $m=10$, reports the term energies from this approximation. Comparing these with the Zeippen *et al.* values as well as with observation we see that the present ${}^1S$ value is in much better agreement with observation and the ${}^1D$ somewhat better. Also apparent is the fact that the inclusion of correlation outside the complex has improved the term energy separation substantially. For our most accurate calculation (the second in Table II) the error in the ${}^1S$ energy is less than 0.8% whereas the error in the ${}^1D$ energy is 2.2%.

As a final check, we have included the term splittings reported by Moser and Nesbet[10] from a Bethe-Goldstone calculation. Some correlation with $1s$ was included in their work and so their total energies are somewhat lower than ours (-74.9920 vs -74.9419 a.u. for ${}^3P$), but the term splittings are not in as good agreement with observation as our present, extensive calculations. As Z increases, the importance of correlation outside the complex decreases. In Table III some transition energies (in emission) are reported, transition energies that enter into the forbidden transitions to be considered later. As Z increases, the Lamb shift also becomes more important. The Cheng *et al.* values reported in Table III include the Breit correction but not the Lamb shift. Rather than correct all the theoretical values for the Lamb shift, the observed values (predicted by Edlén[4]) have been modified so as to remove the Lamb shift. These values are reported in parentheses.

Let us consider the ${}^1S_0$-${}^3P_2$ transition energy first. The present results for the complex, where the number of configurations is $m=4$, are in agreement to within 1% of the MCDHF values for Z less than about 25, but for larger Z

TABLE I. Multiconfiguration Breit-Pauli excitation energies (in cm^{-1}) from the $(2s^22p^4)^3P_2$ ground state of oxygenlike ions for different wave-function expansion lengths m.

	$(2s^22p^4)^3P_1$		$(2s^22p^4)^3P_0$		$(2s^22p^4)^1D_2$		$(2s^22p^4)^1S_0$	
Z	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$
8	165	157	237	225	17 786	17 067	32 378	34 256
9	384	338	501	485	22 917	22 137	42 865	45 419
10	651	637	934	911	27 959	27 124	53 302	56 254
11	1115	1097	1592	1562	33 016	32 134	63 778	66 284
12	1792	1771	2538	2501	38 149	37 233	74 359	77 730
13	2740	2717	3842	3798	43 417	42 477	85 109	88 581
14	4029	4007	5574	5526	48 878	47 927	96 104	99 626
15	5737	5723	7807	7759	54 602	53 653	107 438	110 960
16	7956	7957	10 612	10 569	60 669	59 741	119 229	122 699
17	10 789	10 819	14 051	14 019	67 177	66 291	131 626	134 986
18	14 351	14 429	18 175	18 160	74 237	73 423	144 816	148 000
19	18 775	18 926	23 016	23 019	81 981	81 277	159 031	161 965
20	24 202	24 541	28 580	28 892	90 560	90 607	174 557	179 705
21	30 791	31 320	34 845	35 309	100 140	100 391	191 735	197 142
22	38 711	39 503	41 755	42 404	110 905	111 435	210 963	216 724
23	48 143	49 290	49 223	50 086	123 053	123 956	232 693	238 941
24	59 280	60 896	57 140	58 239	136 792	138 186	257 421	264 336
25	72 321	74 548	65 382	66 731	152 343	154 374	285 675	293 493
26	87 476	90 486	73 827	75 428	169 932	172 776	317 996	327 017
27	104 962	108 962	82 368	84 213	189 789	193 660	354 927	365 521
28	125 000	130 237	90 916	92 989	212 154	217 304	397 002	409 616
29	147 820	154 587	99 410	101 690	237 265	243 996	444 743	459 909
30	173 659	182 299	107 811	110 273	265 370	274 032	498 661	517 000
36	406 155	437 033	155 945	158 884	511 214	542 641	980 377	1 037 261
42	814 839	902 347	201 865	203 721	932 991	1 021 967	1 818 234	1 973 486

there is an increasing difference. The additional correlation in calculations with $m \geq 90$ has produced a marked improvement in agreement with observation, and for $Z \geq 25$, the discrepancy between the present results and the modified observed values is about 1%. For $Z \geq 25$, the most accurate values are the relativistic MCDHF values.

Now let us consider the $^1D_2$-$^3P_0$ transition energy. Again, for $Z < 25$ there is generally good agreement between the present $m=4$ results for the complex and the MCDHF values of Cheng *et al.* However, extensive correlation calculations have produced only a modest improvement in the agreement with observation. In neon, for example, where $Z=10$, correlation has yielded a correction of 813 cm^{-1} when a correction of 2105 cm^{-1} was needed. Thus the additional 86 configurations in the expansion have captured only about 40% of the needed correction. Even so, up to about $Z=18$, the present results with $m \geq 90$ are the best theoretical transition energies.

TABLE II. Comparison of the nonrelativistic energy separation (in a.u.) for oxygen with other theory and observation.

	^1D-^3P	^1S-^3P
Present work: $m=4$	0.0807	0.1437
Present work: $m \geq 90$	0.0735	0.1524
Present work: $m=10$	0.0590	0.1562
Zeippen *et al.*: $m=10$[a]	0.0858	0.1706
Moser and Nesbet[b]	0.0760	0.1606
Observation	0.0719	0.1536

[a] Reference 9.

[b] Reference 10.

The discrepancy in the $^1D_2$ energy level is reflected in other transition energies such as $^1S_0$-$^1D_2$. Again, the present results with $m=4$ are in general agreement with the MCDHF results and there is substantial improvement in the agreeement with observation for all Z when more correlation is included. This transition in oxygen was recently investigated by Chung *et al.*[11] using a nonrelativistic MCHF wave function. Whereas the MCHF + BP programs assume a single orthonormal orbital basis, the MCHF programs permit multiple orbitals of the same type as well as different orbitals for the inital and final states. Much shorter expansions (15 configuration states for ^1S, 21 for ^1D) yielded a transition energy of 18 977 cm^{-1}, which is too large by 1052 cm^{-1} whereas the present nonrelativistic value was too small by -597 cm^{-1}. This comparison shows the difficulty in predicting such term splittings accurately.

At this point it should be mentioned that Cheng *et al.*[12] in a more recent publication, have estimated corrections to transition energies between terms, using results from Z-dependent perturbation theory. These have not been included in the present tables since the corrections do not

TABLE III. Multiconfiguration Breit-Pauli energy separation (in cm^{-1}) in the oxygen sequence for the complex ($m=4$) and for correlation outside the complex ($m \geq 90$), compared with results from other theories and observation.

	Present		Cheng		
Z	$m=4$	$m \geq 90$	*et al.*[a]	Observation[b]	
		(a) $^1S_0$-$^3P_2$			
8	32 378	34 256		33 793	
9	42 865	45 419		44 918	
10	53 302	56 254	52 672	55 751	(55 686)
11	63 778	66 984	63 104	66 496	(66 399)
12	74 359	77 730	73 655	77 287	(77 151)
14	96 104	99 626	95 382	99 343	(99 107)
16	119 229	122 699	118 546	122 700	(122 336)
18	144 816	148 000	144 262	148 513	(148 000)
20	174 557	179 705	174 282	178 568	(177 892)
25	285 675	293 493	287 654	291 899	(290 445)
30	498 661	517 000	508 216	512 557	(509 956)
		(b) $^1S_0$-$^1D_2$			
8	14 592	17 189		17 925	
9	19 949	23 282		24 045	
10	25 343	29 131	24 825	29 910	(29 846)
11	30 763	34 850	30 214	35 655	(35 567)
12	36 210	40 497	35 648	41 362	(41 227)
14	47 226	51 699	46 692	52 775	(52 542)
16	58 560	62 958	58 121	64 405	(64 047)
18	70 579	74 576	70 323	76 679	(76 178)
20	83 997	89 098	84 036	90 366	(89 710)
25	133 332	139 119	135 078	141 048	(139 654)
30	233 291	242 968	239 735	245 232	(242 780)
		(c) $^1D_2$-$^3P_0$			
8	17 549	16 842		15 641	
9	22 416	21 652		20 383	
10	27 025	26 213	27 036	24 920	
11	31 424	30 572	31 421	29 265	
12	35 611	34 731	35 592	33 404	
14	43 305	42 400	43 238	41 000	
16	50 057	49 173	49 921	47 647	
18	56 062	55 264	55 833	53 527	
20	61 980	61 715	61 656	59 322	
25	86 962	87 643	86 865	84 346	(85 905)
30	157 559	163 759	159 937	156 888	(159 623)

[a] Reference 3.

[b] Edlén (Ref. 4). The values in parentheses have been modified to exclude the Lamb shift.

affect the quality of the wave function. However, it is enlightening to consider these second-order corrections which are constants, independent of Z. For the $^1S_0$-$^3P_2$ transition, Cheng *et al.*[12] estimate the second-order correlation from outside the complex to be 5400 cm^{-1}. When added to the complex to the $m=4$ or Cheng *et al.*[3] results reported in Table III, this correction improves the transition energy, but overestimates the correction. Similar corrections for the $^1D_2$-$^3P_0$ and $^1S_0$-$^1D_2$ transitions are -2300 cm^{-1} and 7700 cm^{-1}, respectively. The negative correction to the $^1D_2$-$^3P_0$ transition energy indicates that there is more correlation outside the complex in the ^1D state than in the ^3P state. The modest improvement in the accuracy of this transition energy suggests that any further improvement would require that special attention be given to correlation in the ^1D state.

B. Fine-structure splitting

The fine-structure splitting depends primarily on the relativistic corrections (in the nonrelativistic limit all the levels of the term have the same energy) but also to some extent on correlation.

In Table IV we compare the $^3P_0$-$^3P_2$ energy separation

TABLE IV. Comparision of $2p^4(^3P_0\text{-}^3P_2)$ multiconfiguration Breit-Pauli energy separations (in cm^{-1}) in the oxygen sequence with other theory and observation. The values in parentheses in the observed column have been modified to exclude the Lamb shift.

Z	Ion	Present $m=4$	 $m\geq 90$	Cheng *et al.*[a]	Observed[b]	
8	O	237	225		227	
9	F 1+	501	485		490	
10	Ne 2+	934	911	811	921	
12	Mg 4+	2538	2501	2415	2521	
14	Si 6+	5574	5526	5452	5568	(5564)
16	S 8+	10 612	10 569	10 504	10 648	(10 640)
18	Ar 10+	18 175	18 160	18 106	18 307	(18 293)
20	Ca 12+	28 580	28 892	28 590	28 880	(28 861)
25	Mn 17+	65 382	66 731	65 711	66 505	(64 881)
30	Zn 22+	107 811	110 273	108 544	110 437	(107 553)

[a] Reference 3.
[b] Edlén (Ref. 4).

of both the complex and correlation approximations with the values reported by Cheng *et al.*[3] For low Z, correlation has tended to bring results into better agreement with observation, but overcorrects the complex values. For $Z=20$ (where 125 configurations were included in the expansion) the results are in excellent agreement with observation. Comparing the present results for the complex with those reported by Cheng *et al.*, we see that they are similar (to within 1%) for $Z>18$, but that there is an increasing difference as Z decreases. The inclusion of correlation beyond the complex has improved the fine-structure splitting at the lower Z values, but for $Z>25$ the $m=4$ results are in better agreement with observation when the Lamb shift is taken into account.

To the extent that energy differences may be used as a criterion for accuracy, the analysis of term-energy splitting as well as fine-structure splitting indicate that the present wave function with $m\geq 90$ is the most reliable for $Z\leq 20$ and that for $Z\geq 25$, higher-order relativistic effects are entering that cannot be accounted for in the MCHF + BP formalism.

C. Transition probabilities

In Table V, MCHF + BP transition probabilities are reported for some forbidden electric quadrupole ($E2$) transitions in the oxygen isoelectronic sequence and in Table VI, transition probabilities for some forbidden magnetic dipole ($M1$) transitions. All values are in cm^{-1}.

Transition probabilities are defined as

$$A(E2)=\frac{1.120\times 10^{18}}{\omega_i\lambda^5}S_{E2}\ ,$$

$$A(M1)=\frac{2.6971\times 10^{13}}{\omega_i\lambda^3}S_{M1}\ ,$$

where λ is the transition wavelength in angstroms, ω_i is the statistical weight of the initial state, and S_{E2} and S_{M1} are the electric quadrupole and magnetic dipole line strengths, respectively.

The values reported in Tables V and VI were all based on the theoretical wavelengths or, equivalently, theoretical transition energies (recall that $1/\lambda$ is proportional to the transition energy). Clearly, because the transition probability is the product of a line strength and a transition energy raised to a power, any error in the transition energy will be magnified as an error in the transition probability. This accounts for much of the difference in the $m=4$ and $m\geq 90$ results. In order to obtain a better understanding of the effect of correlation on the transition probability, let us analyze the line strength alone since transition energies already have been considered.

1. Electric quadrupole line strengths

In Table VII we compare line strengths for some $E2$ transitions with similar results reported by Cheng *et al.* The effect of correlation in the MCHF + BP approximation varies from 5—10% in the $^1S_0\text{-}^1D_2$ transition to 30—50% in the $^1D_2\text{-}^3P_0$ transition. The most striking feature is that there now is no clear pattern of agreement with the MCDHF results, though often there is a converging trend for higher Z. The $^1D_2\text{-}^3P_2$ is a case in point. For neon ($Z=10$) there are large relative differences between the three values but for $Z\geq 20$, the differences are of the order of a few percent. In $E2$ transitions, s-d transitions between the configuration states of the initial and final L,S,J state are allowed. Such contributions arise from correlation outside the complex and hence their significance decreases as Z increases. Neither the present $m=4$ nor the Cheng *et al.* results include these contributions. Some line strengths reported by Garstang[13] using Hartree-Fock functions and a semiempirical method for including spin-orbit interaction, have also been tabulated. Because of the lack of sensitivity of the line strength on the details of the wave function, these results are more accurate than one might expect.

TABLE V. Multiconfiguration Breit-Pauli transition probabilities for the forbidden $E2$ transition in the oxygen sequence for two different wave-function expansion lengths m. Numbers in parentheses denote power of ten: (-11) means 10^{-11}.

	$^3P_1$-$^3P_2$		$^3P_0$-$^3P_2$		$^1D_2$-$^3P_2$		$^1S_0$-$^3P_2$		$^1S_0$-$^1D_2$		$^1D_2$-$^3P_1$		$^1D_2$-$^3P_0$	
Z	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$
8	1.58(−11)	1.743(−11)	1.305(−10)	1.409(−10)	3.217(−5)	3.327(−5)	1.510(−4)	2.250(−4)	4.446(−1)	1.057	4.387(−6)	5.370(−6)	2.604(−6)	1.197(−6)
9	2.464(−10)	2.608(−10)	2.026(−9)	2.110(−9)	1.155(−4)	1.135(−4)	6.607(−4)	1.029(−3)	7.792(−1)	1.724	1.528(−5)	1.694(−5)	8.247(−6)	4.204(−6)
10	2.590(−9)	2.706(−9)	2.102(−8)	2.164(−8)	3.438(−4)	3.328(−4)	2.244(−3)	3.415(−3)	1.194	2.422	4.367(−5)	4.650(−5)	2.207(−5)	1.217(−5)
11	2.025(−8)	2.106(−8)	1.602(−7)	1.644(−7)	8.899(−4)	8.580(−4)	6.314(−3)	9.310(−3)	1.669	3.132	1.071(−4)	1.118(−4)	5.185(−5)	3.055(−5)
12	1.260(−7)	1.310(−7)	9.613(−7)	9.863(−7)	2.072(−3)	2.000(−3)	1.541(−2)	2.204(−2)	2.195	3.852	2.330(−4)	2.405(−4)	1.100(−4)	6.862(−5)
13	6.557(−7)	6.830(−7)	4.759(−6)	4.890(−6)	4.449(−3)	4.307(−3)	3.369(−2)	4.685(−2)	2.766	4.579	4.600(−4)	4.715(−4)	2.146(−4)	1.409(−4)
14	2.952(−6)	3.086(−6)	2.012(−5)	2.072(−5)	8.965(−3)	8.718(−3)	6.734(−2)	9.132(−2)	3.383	5.317	8.354(−4)	8.543(−4)	3.911(−4)	2.689(−4)
15	1.180(−5)	1.240(−5)	7.444(−5)	7.689(−5)	1.719(−2)	1.681(−2)	1.251(−1)	1.658(−1)	4.051	6.073	1.416(−3)	1.446(−3)	6.731(−4)	4.828(−4)
16	4.271(−5)	4.511(−5)	2.456(−4)	2.545(−4)	3.169(−2)	3.118(−2)	2.183(−1)	2.829(−1)	4.783	6.856	2.258(−3)	2.304(−3)	1.105(−3)	8.246(−4)
17	1.420(−4)	1.510(−4)	7.329(−4)	7.612(−4)	5.669(−2)	5.614(−2)	3.612(−1)	4.577(−1)	5.602	7.685	3.409(−3)	3.482(−3)	1.743(−3)	1.353(−3)
18	4.389(−4)	4.701(−4)	1.998(−3)	2.079(−3)	9.905(−2)	9.884(−2)	5.700(−1)	7.057(−1)	6.543	8.589	4.905(−3)	5.014(−3)	2.667(−3)	2.151(−3)
19	1.272(−3)	1.373(−3)	5.016(−3)	5.221(−3)	1.700(−1)	1.711(−1)	8.626(−1)	1.041	7.663	9.613	6.753(−3)	6.916(−3)	3.993(−3)	3.353(−3)
20	3.481(−3)	3.852(−3)	1.166(−2)	1.277(−2)	2.882(−1)	2.994(−1)	1.257	1.587	9.051	1.213(+1)	8.937(−3)	9.579(−3)	5.910(−3)	5.430(−3)
21	9.050(−3)	1.013(−2)	2.523(−2)	2.787(−2)	4.839(−1)	5.065(−1)	1.771	2.225	1.084(+1)	1.422(+1)	1.141(−2)	1.221(−2)	8.739(−3)	8.169(−3)
22	2.245(−2)	2.541(−2)	5.092(−2)	5.671(−2)	8.075(−1)	8.521(−1)	2.419	3.027	1.324(+1)	1.702(+1)	1.411(−2)	1.508(−2)	1.306(−2)	1.244(−2)
23	5.331(−2)	6.110(−2)	9.616(−2)	1.079(−1)	1.341	1.429	3.212	4.007	1.656(+1)	2.092(+1)	1.695(−2)	1.809(−2)	1.995(−2)	1.942(−2)
24	1.217(−1)	1.412(−1)	1.704(−1)	1.925(−1)	2.220	2.390	4.159	5.176	2.129(+1)	2.649(+1)	1.985(−2)	2.116(−2)	3.141(−2)	3.136(−2)
25	2.675(−1)	3.145(−1)	2.843(−1)	3.229(−1)	3.666	3.991	5.266	6.541	2.820(+1)	3.464(+1)	2.273(−2)	2.420(−2)	5.129(−2)	5.269(−2)
26	5.680(−1)	6.769(−1)	4.481(−1)	5.109(−1)	6.034	6.651	6.540	8.110	3.848(+1)	4.681(+1)	2.552(−2)	2.714(−2)	8.695(−2)	9.222(−2)
27	1.168	1.411	6.704(−1)	7.662(−1)	9.902	1.106(+1)	7.988	9.892	5.400(+1)	6.525(+1)	2.818(−2)	2.994(−2)	1.525(−1)	1.674(−1)
28	2.329	2.853	9.570(−1)	1.095	1.619(+1)	1.834(+1)	9.622	1.190(+1)	7.765(+1)	9.348(+1)	3.066(−2)	3.256(−2)	2.750(−1)	3.130(−1)
29	4.515	5.613	1.310	1.498	2.634(+1)	3.028(+1)	1.146(+1)	1.415(+1)	1.140(+2)	1.371(+2)	3.295(−2)	3.497(−2)	5.054(−1)	5.967(−1)
30	8.524	1.076(+1)	1.730	1.975	4.264(+1)	4.977(+1)	1.351(+1)	1.666(+1)	1.700(+2)	2.048(+2)	3.505(−2)	3.719(−2)	9.384(−1)	1.149
36	2.425(+2)	3.379(+2)	5.469	6.083	6.642(+2)	8.589(+2)	3.185(+1)	3.774(+1)	2.109(+3)	2.662(+3)	4.383(−2)	4.673(−2)	3.388(+1)	5.053(+1)
42	3.776(+3)	5.916(+3)	1.085(+1)	1.142(+1)	7.746(+3)	1.127(+4)	6.222(+1)	5.945(+1)	2.334(+4)	3.195(+4)	4.794(−2)	5.198(−2)	7.095(+2)	1.265(+3)

TABLE VI. Multiconfiguration Breit-Pauli transition probabilities for the forbidden $M1$ transitions in the oxygen sequence for different wave-function expansion lengths m.

	$^3P_0$-$^3P_1$		$^1D_2$-$^3P_2$		$^1D_2$-$^3P_1$		$^1S_0$-$^3P_1$		$^3P_1$-$^3P_2$	
Z	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$	$m=4$	$m\geq 90$
8	2.047(−5)	1.705(−5)	7.476(−3)	7.023(−3)	2.424(−3)	2.278(−3)	7.182(−2)	7.789(−2)	1.001(−4)	8.702(−5)
9	1.927(−4)	1.702(−4)	4.413(−2)	4.192(−2)	1.405(−2)	1.335(−2)	4.353(−1)	4.693(−1)	9.505(−4)	8.680(−4)
10	1.223(−3)	1.112(−3)	1.911(−1)	1.831(−1)	5.937(−2)	5.684(−2)	1.919	2.056	6.198(−3)	5.809(−3)
11	5.840(−3)	5.409(−3)	6.696(−1)	6.463(−1)	2.014(−1)	1.942(−1)	6.807	7.253	3.116(−2)	2.972(−2)
12	2.241(−2)	2.102(−2)	2.008	1.952	5.800(−1)	5.627(−1)	2.057(+1)	2.184(+1)	1.292(−1)	1.249(−1)
13	7.196(−2)	6.806(−2)	5.348	5.232	1.468	1.433	5.501(+1)	5.820(+1)	4.617	4.513
14	1.983(−1)	1.885(−1)	1.296(+1)	1.277(+1)	3.347	3.284	1.335(+2)	1.409(+2)	1.466	1.447
15	4.759(−1)	4.533(−1)	2.913(+1)	2.886(+1)	6.989	6.892	2.992(+2)	3.154(+2)	4.226	4.211
16	1.002	9.529(−1)	6.149(+1)	6.134(+1)	1.354(+1)	1.341(+1)	6.284(+2)	6.616(+2)	1.124(+1)	1.130(+1)
17	1.849	1.745	1.233(+2)	1.238(+2)	2.455(+1)	2.444(+1)	1.249(+3)	1.314(+3)	2.794(1)	2.834(+1)
18	2.956	2.745	2.367(+2)	2.393(+2)	4.202(+1)	4.201(+1)	2.370(+3)	2.491(+3)	6.547(+1)	6.700(+1)
19	3.996	3.592	4.380(+2)	4.460(+2)	6.828(+1)	6.856(+1)	4.318(+3)	4.535(+3)	1.458(+2)	1.505(+2)
20	4.339	4.263	7.856(+2)	8.084(+2)	1.059(+2)	1.074(+2)	7.597(+3)	8.098(+3)	3.101(+2)	3.198(+2)
21	3.388	3.230	1.372(+3)	1.421(+3)	1.574(+2)	1.601(+2)	1.300(+4)	1.384(+4)	6.331(+2)	6.581(+2)
22	1.403	1.215	2.340(+3)	2.443(+3)	2.252(+2)	2.296(+2)	2.150(+4)	2.302(+4)	1.246(+2)	1.305(+3)
23	6.100(−2)	2.446(−2)	3.912(+3)	4.116(+3)	3.112(+2)	3.179(+2)	3.482(+4)	3.738(+4)	2.370(+3)	2.503(+3)
24	1.530(−1)	2.930(−1)	6.420(+3)	6.813(+3)	4.171(+2)	4.267(+2)	5.517(+4)	5.942(+4)	4.371(+3)	4.654(+3)
25	5.025	7.184	1.037(+4)	1.110(+4)	5.436(+2)	5.569(+2)	8.574(+4)	9.265(+4)	7.833(+3)	8.409(+3)
26	3.666(+1)	4.917(+1)	1.649(+4)	1.782(+4)	6.912(+2)	7.089(+2)	1.310(+5)	1.421(+5)	1.367(+4)	1.480(+4)
27	1.589(+2)	2.083(+2)	2.587(+4)	2.824(+4)	8.598(+2)	8.827(+2)	1.971(+5)	2.147(+5)	2.328(+4)	2.542(+4)
28	5.200(+2)	6.760(+2)	4.006(+4)	4.418(+4)	1.049(+3)	1.078(+3)	2.926(+5)	3.202(+5)	3.874(+4)	4.267(+4)
29	1.419(+3)	1.842(+3)	6.128(+4)	6.829(+4)	1.258(+3)	1.294(+3)	4.294(+5)	4.722(+5)	6.313(+4)	7.017(+4)
30	3.404(+3)	4.426(+3)	9.263(+4)	1.044(+5)	1.487(+3)	1.531(+3)	6.236(+5)	6.897(+5)	1.009(+5)	1.132(+5)
36	1.462(+5)	1.983(+5)	8.854(+5)	1.075(+6)	3.228(+3)	3.350(+3)	4.909(+6)	5.679(+6)	1.195(+6)	1.425(+6)
42	1.842(+6)	2.687(+6)	6.131(+6)	8.125(+6)	5.521(+3)	5.812(+3)	3.023(+7)	3.716(+7)	9.142(+6)	1.172(+7)

TABLE VII. Comparison of line strengths for some $E2$ transitions in the oxygen sequence.

	Present		Cheng	
Z	$m = 4$	$m \geq 90$	*et al.*[a]	Garstang[b]
		(a) $^1S_0$-$^1D_2$		
8	6.00	6.293		6.47
9	2.203	2.251		2.33
10	1.020	1.031	1.064	1.05
12	3.149(−1)	3.158(−1)	3.239(−1)	
14	1.286(−1)	1.286(−1)	1.311(−1)	
16	6.203(−2)	6.190(−2)	6.277(−2)	
18	3.336(−2)	3.325(−2)	3.352(−2)	
20	1.933(−2)	1.929(−2)	1.927(−2)	
25	5.976(−3)	5.936(−3)	5.819(−3)	
30	2.197(−3)	2.160(−3)	2.092(−3)	
42	3.833(−4)	3.658(−4)	3.482(−4)	
		(b) $^1S_0$-$^3P_2$		
8	3.790(−5)	4.260(−5)		
9	4.077(−5)	4.752(−5)		
10	4.658(−5)	5.414(−5)	5.786(−5)	
11	5.343(−5)	6.165(−5)	6.777(−5)	
12	6.054(−5)	6.937(−5)	7.644(−5)	
14	7.335(−5)	8.309(−5)	9.031(−5)	
16	8.092(−5)	9.085(−5)	9.706(−5)	
18	7.992(−5)	8.876(−5)	9.360(−5)	
20	6.928(−5)	7.562(−5)	7.935(−5)	
25	2.472(−5)	2.682(−5)	2.721(−5)	
30	3.914(−6)	4.029(−6)	4.531(−6)	
42	2.796(−8)	1.773(−8)	6.911(−8)	
		(c) $^1D_2$-$^3P_0$		
8	6.985(−5)	3.944(−5)		
9	6.507(−5)	3.944(−5)		
10	6.835(−5)	4.392(−5)	2.380(−7)	
11	7.556(−5)	5.107(−5)	2.200(−5)	
12	8.573(−5)	6.062(−5)	5.077(−5)	
14	1.147(−4)	8.761(−5)	1.048(−4)	
16	1.569(−4)	1.281(−4)	1.624(−4)	
18	2.150(−4)	1.863(−4)	2.321(−4)	
20	2.885(−4)	2.708(−4)	3.149(−4)	
25	4.605(−4)	4.550(−4)	4.908(−4)	
30	4.315(−4)	4.356(−4)	4.356(−4)	
42	1.516(−4)	1.540(−4)	1.404(−4)	
		(d) $^1D_2$-$^3P_2$		
8	8.071(−4)	1.026(−3)		
9	8.158(−4)	9.531(−4)		
10	8.985(−4)	1.012(−3)	1.596(−3)	
11	1.013(−3)	1.118(−3)	1.495(−3)	
12	1.145(−3)	1.248(−3)	1.529(−3)	
14	1.435(−3)	1.539(−3)	1.735(−3)	
16	1.722(−3)	1.829(−3)	1.986(−3)	
18	1.961(−3)	2.068(−3)	2.197(−3)	
20	2.113(−3)	2.189(−3)	2.315(−3)	
25	1.995(−3)	2.032(−3)	2.088(−3)	
30	1.447(−3)	1.438(−3)	1.457(−3)	
42	4.892(−4)	4.515(−4)	4.572(−4)	

[a] Reference 3.

[b] Reference 11.

2. *Magnetic dipole line strengths*

The line strengths for magnetic dipole ($M1$) transitions $^3P_1$-$^3P_2$ and $^1S_0$-$^3P_1$ are compared in Table VIII. In the case of the former, the effect of correlation outside the complex is negligible and relativistic effects only begin to show up for $Z \geq 30$. In the case of $^1S_0$-$^3P_1$, which is a transition between different terms, the effect of correlation is somewhat larger—8% in Mg ($Z=12$), for example. Again, as observed in $E2$ transitions, as Z increases, all three line strengths are becoming more similar.

3. *Observation*

The only transitions where some results derived from observation are available are the $^1S_0$-$^1D_2$ transition in oxygen identified as the 5577-Å line and the $^1S_0$-$^3P_1$ transition yielding the 2972-Å line. The former line is a key spectral feature in the study of auroras. It has also been observed in the solar spectrum and measurements of its intensity have been used to determine the abundance of oxygen in the sun. The upper level may also decay via the $M1$ transition to the $^3P_1$ state. The relative intensities of these two lines provides information about the ratio of the transition probabilities. Omholt[14] studied several types of auroras and estimated an upper limit of $\tau = 0.75$ sec for the $^1S_0$ state. LeBlanc *et al.*[15] studied the emission of several forbidden lines in oxygen and found the ratio of intensities of the 5577 to 2972 Å lines to be 22±2. On the other hand, McConkey *et al.*[16] measured the ratio in the laboratory and obtained the result of 18.6±3.7. Kernahan and Pang measured the $^1S_0$-$^1D_2$ transition probabilty as well as the intensity ratio of the two lines. This data predicts a lifetime of 0.905 sec which appears to be too

TABLE VIII. Comparison of some line strengths for $M1$ transitions in the oxygen sequence.

	Present		Cheng
Z	$m=4$	$m \geq 90$	*et al.*[a]
	(a)	$^3P_1$-$^3P_2$	
8	2.500	2.500	
9	2.500	2.500	
10	2.500	2.499	2.499
11	2.499	2.499	2.498
12	2.498	2.498	2.497
14	2.493	2.493	2.491
16	2.483	2.482	2.479
18	2.464	2.462	2.457
20	2.433	2.431	2.422
25	2.303	2.297	2.282
30	2.143	2.132	2.112
42	1.880	1.870	1.839
	(b)	$^1S_0$-$^3P_1$	
8	7.966(−5)	7.284(−5)	
9	2.100(−4)	1.899(−4)	
10	4.876(−4)	4.431(−4)	6.109(−4)
11	1.026(−3)	9.403(−4)	1.257(−3)
12	1.996(−3)	1.847(−3)	2.401(−3)
14	6.339(−3)	5.975(−3)	7.418(−3)
16	1.691(−2)	1.624(−2)	1.943(−2)
18	3.957(−2)	3.875(−2)	4.484(−2)
20	8.287(−2)	8.037(−2)	9.278(−2)
25	3.273(−1)	3.273(−1)	3.537(−1)
30	6.735(−1)	6.820(−1)	7.015(−1)
42	1.110	1.121	1.113

[a] Reference 3.

TABLE IX. Comparison of some results for oxygen.

	$A(^1S_0$-$^1D_2)$	$A(^1S_0$-$^3P_1)$	Ratio	$\tau(^1S_0)$ (sec)
Theory				
(1) Present				
$m=4$	1.244	0.0829	15.0	0.754
$m \geq 90$	1.304	0.0758	17.2	0.725
(2) MCHF[a]	1.22			
(3) NCMET[b]	1.183			
(4) Garstang[c]	1.28			
Experiment	1.06±0.32[d]	(0.045)[d]	23.7[d]	(0.905)[d]
			22±2[e]	0.76[g]
			18.6±3.7[f]	0.70[h]
				0.67[i]

[a] Chung *et al.* (Ref. 11).

[b] Nicolaides *et al.* (Ref. 18).

[c] Garstang (Ref. 13).

[d] Kernahan and Pang (Ref. 17). Reults in parentheses are deduced values.

[e] Le Blanc *et al.* (Ref. 15).

[f] McConkey *et al.* (Ref. 16).

[g] Corney and Williams (Ref. 19).

[h] Omholt (Ref. 14).

[i] Evans and Jones (Ref. 20).

large. (A review of the importance of this line in astrophysics and various attempts to determine the lifetime of the $^1S_0$ state may be found in the paper by Chung *et al.*[11]) In Table IX, we have summarized all the available data. All theoretical values are now computed using the observed transition energies. The present correlation result with $m \geq 90$ yields a ratio of intensities in agreement with the McConkey *et al.* ratio. In fact, of all the theoretical predictions it has the largest ratio. The lifetime of 0.725 sec also satisfies the upper limit requirement of 0.75 sec. It would appear that the nonrelativistic $E2$ transition probability obtained by Nicolaides *et al.* using a nonclosed shell many-electron theory (NCMET) has yielded a value that is too small, and that the nonrelativistic MCHF value is also too small. The present value of 1.304 sec^{-1} is in the middle of the (1.24—1.37) sec^{-1} range "deduced" by Chung *et al.* from observed data.

IV. CONCLUSION

Our extensive study of term splitting, fine structure splitting, and transition probabilities using the MCHF + BP approximation, has shown that correlation outside the complex is important for transitions between terms, at least for $Z \leq 20$. Since the transition probabilities are proportional to the transition energy raised to the power 5 in the case of an $E2$ transition, and 3 in the case of an $M1$ transition, relatively small changes in the transition energy results in fairly large changes in the transition probability. For example, a 10% increase in the transition energy will increase the transition probability of an $E2$ transition by a factor of 1.61. At least in the range $Z \leq 20$, the present $m \geq 90$ results predict transition energies more accurately than any other theory, and we conclude that in this region, the line strength is also more accurate. In this connection, it should be mentioned that Kastner *et al.*[5] have reported some transition probabilities for some of the transitions considered here. Their calculations were based on Thomas-Fermi-Dirac orbitals and their wave-function expansion included some configurations outside the complex. In general, their results were similar to the present $m = 4$ results, but only transition probabilities were reported and it was not clear whether these were based on observed or theoretical transition energies. As a result, their values have not been included in the analysis.

ACKNOWLEDGMENT

This research was supported by a grant from the Office of Basic Energy Science, U.S. Department of Energy.

---

[1] D. E. Osterbrock, *Astrophysics of Gaseous Nebulae* (Freeman, San Francisco, 1974).

[2] E. Hinnov and S. Suckewer, Phys. Lett. 79A, 298 (1980).

[3] K. T. Cheng, Y-K. Kim, and J. P. Desclaux, At. Data Nucl. Data Tables 24, 111 (1979).

[4] B. Edlén, Phys. Scr. 28, 51 (1983).

[5] S. O. Kastner, A. K. Bhatia, and L. Cohen, Phys. Scr. 15, 259 (1977).

[6] W. Eissner, M. Jones, and H. Nussbaumer, Comput. Phys. Commun. 8, 270 (1972).

[7] C. Froese Fischer, Comput. Phys. Commun. 14, 145 (1978).

[8] C. Froese Fischer, J. Phys. B 16, 157 (1983).

[9] C. J. Zieppen, M. J. Seaton, and D. C. Morton, Mon. Not. R. Astron. Soc. 181, 527 (1977).

[10] C. M. Moser and R. K. Nesbet, Phys. Rev. A 4, 1336 (1971); 6, 1710 (1972).

[11] S. Chung, C. C. Lin, C. Froese Fischer, and E. T. P. Lee, J. Chem. Phys. 76, 498 (1982).

[12] K. T. Cheng, C. Froese Fischer, and Y-K. Kim, J. Phys. B 15, 181 (1982).

[13] R. H. Garstang, Mon. Not. R. Astron. Soc. 111, 115 (1951).

[14] A. Omholt, in *The Airglow and the Aurorae* edited by E. B. Armstrong and A. Dalgarno (Pergamon, London, 1956).

[15] F. S. Leblanc, O. Oldenberg, and N. P. Carleton, J. Chem. Phys. 45, 2200 (1966).

[16] J. W. McConkey, D. J. Burns, K. A. Moran, and K. G. Emeleus, Phys. Lett. 22, 416 (1966).

[17] J. A. Kernahan and P. H.-L. Pang, Can. J. Phys. 53, 455 (1975).

[18] C. Nicolaides, O. Sinanŏglu, and P. Westhaus, Phys. Rev. A 4, 1400 (1971).

[19] A. Corney and O. M. Williams, J. Phys. B 5, 686 (1972).

[20] W. F. J. Evans and A. Vallance Jones, Can. J. Phys. 43, 697 (1965).