

## Oscillator strengths for the transitions in Ca XIII

K. S. Baliyan and A. K. Bhatia

*Laboratory for Astronomy and Solar Physics, NASA Goddard Space Flight Center, Greenbelt, Maryland 20771*

(Received 4 January 1993)

The absorption oscillator strengths for a number of transitions among  $LS$  states and the fine-structure levels calculated using extensive configuration interaction in the wave functions are reported. The relativistic results are obtained adopting an intermediate-coupling scheme through the use of the terms of the Breit-Pauli Hamiltonian. In general, there is very good agreement between length and velocity forms of the oscillator strengths and the energies obtained using these wave functions compare very well with the observed values. The comparison of the oscillator strengths calculated in the present work with the other available calculations shows good agreement. Also reported are accurate results for many astrophysically important transitions involving quintet states. It is noted that spin-spin and spin-other-orbit terms of the Breit-Pauli Hamiltonian have considerable effect on the  $f$  values for the intercombination transitions.

PACS number(s): 32.70.Cs, 31.20.Di, 31.20.Tz, 31.30.Jv

### I. INTRODUCTION

Accurate oscillator strengths and transition probabilities for the transitions in the cosmically abundant ions of oxygen isoelectronic sequence are required for a detailed study of the celestial bodies. Highly ionized ions of this sequence are also of particular interest for the fusion research and modeling of plasmas. A limited amount of effort is devoted to the calculation of oscillator strengths, energy levels, and transition probabilities for some ions of this sequence, by Saraph, Seaton, and Shemming [1], Pradhan [2], Mason [3], Bhatia, Feldman, and Doshek [4], Butler and Mendoza [5], Reed and Henry [6], Cowan [7], Cheng, Kim, and Desclaux [8], Baluja and Zeippen [9], Fawcett [10], Tayal and Henry [11], Hibbert *et al.* [12], and references therein. The most important member of this sequence, namely, neutral oxygen, has attracted much attention and relatively less work concerns other ions of this sequence. The existing data are sparse and mostly pertain to transitions among the levels of  $n=2$  complex. Further, most of the data are obtained with very limited, if at all, electron correlations.

The transitions within the ground configuration of highly ionized systems, such as Ca XIII, are of basic importance for coronal studies. Whereas, for diagnostic spectroscopy in fusion plasmas, it is essential to include the  $n=3$  shell transitions at least. This is because of the emphasis on visible spectroscopy and on localizing the vicinity of surfaces from which the impurities are released. In the present work we consider the Ca XIII ion of the oxygen isoelectronic sequence and calculate absorption oscillator strengths for a number of transitions using the configuration-interaction technique (Hibbert [13]). The accurate wave functions are constructed including the electron-correlation effects through extensive configuration interaction. The calculation is performed both in  $LS$  coupling as well as intermediate coupling taking into account the relativistic effects via Breit-Pauli terms of the Hamiltonian. Relatively few calculations are reported

for this ion. Mason [3], Cheng, Kim, and Desclaux [8], Fawcett [10], and Baluja and Zeippen [9] have calculated energy levels, oscillator strengths, and transition probabilities using various techniques. Energy levels and radiative transition probabilities are reported by Mason for the transitions among the  $2s^22p^4$  and  $2s2p^5$  levels using the SUPERSTRUCTURE [14] program. Cheng, Kim, and Desclaux [8] used the multiconfiguration Dirac-Fock (MCDF) technique (Desclaux [15]) to calculate energy levels and oscillator strengths but included configurations within the  $n=2$  complex only. The Hartree-Fock relativistic (HFR) program of Cowan [16] was used by Fawcett [10] including a limited number of configurations from the  $n=3$  complex. He calculated the line oscillator strength between the levels of  $2s^22p^4$ ,  $2s2p^5$ ,  $2p^6$ ,  $2s^22p^33s$ , and  $2s^22p^33d$  configurations. Baluja and Zeippen [9] used  $3s$ ,  $3p$ , and  $3d$  correlation orbitals and reported oscillator strengths between the  $n=2$   $LS$  states. All these calculations, therefore, are for the transitions among  $n=2$  configuration states except the calculation of Fawcett which includes a few levels from the  $n=3$  complex. A systematic calculation which takes account of all the important electron correlation effects is clearly warranted. Further, none of the previous calculations has considered the  $2s^22p^4\ ^3P^e-2s^22p^3\ ^5S^o$  transition which is most suitable for the abundance studies. A detailed study of the transitions involving quintet systems, whether for an understanding of the structure of the stellar atmosphere or for an investigation of heating and radiationless mechanisms in laboratory plasmas, necessarily requires an evaluation of the intercombination oscillator strength. We have calculated  $f$  values for many intercombination lines as well.

### II. CALCULATION

The basic purpose of the present study of the Ca XIII ion is to calculate sufficiently accurate oscillator strengths, excitation collision strengths, and perhaps pho-

toionization cross sections for their use in astrophysical and fusion applications. Since any inaccuracy in the construction of atomic or ionic wave functions enters directly into the collision matrix, it is vital for the accuracy of the final results that wave functions employed are of high quality. In this work we attempt to obtain such wave functions for the states of Ca XIII using the sophisticated configuration-interaction method as implemented in the CIV3 [13] program. In this method the nonrelativistic configuration-interaction wave functions are expressed in the form

$$\Phi_j(LS) = \sum_{i=1}^m a_{ij} \phi_i(\alpha_i LS). \quad (1)$$

For a given set of  $\{\phi_i\}$ , the variationally optimal values of the mixing coefficients  $a_{ij}$  are the components of the eigenvectors of the Hamiltonian matrix. In the above expression, each single-configuration state function  $\{\phi_i\}$  is constructed from one-electron orbitals whose angular momenta are coupled (as described by  $\alpha_i$ ) to form a total  $L$ ,  $S$ , and  $\Pi$ , common to all  $m$  configurations. The radial part of these orbitals is represented as a sum of Slater-type orbitals,

$$P_{nl}(r) = \sum_{i=1}^k c_i r^{p_i} \exp(-\zeta_i r). \quad (2)$$

For the  $1s$ ,  $2s$ , and  $2p$  orbitals, the parameters  $c_i$ ,  $p_i$ , and  $\zeta_i$  are taken as Hartree-Fock values given by Clementi and Roetti [17] for the ground state  $^3P^e$ . The parameters of the rest of the orbitals used in the present calculation for the construction of the wave functions are obtained using the following optimization procedure.

The  $3s$  function parameters are optimized on the energy of the  $2s^2 2p^3 3s^3 S^o$  state. Since the  $3s$  functions appropriate to the  $2s^2 2p^3 3s^5 S^o$  state are substantially different from those for the  $2s^2 2p^3 3s^3 S^o$  state, and since the CIV3 program uses orthogonal orbitals only, it is necessary to introduce another radial function, which we labeled as  $4s$ , so that the  $2s^2 2p^3 3s^5 S^o$  state is represented by a linear combination of  $2s^2 2p^3 3s$  and  $2s^2 2p^3 4s$  configurations. The parameters for the  $4s$  orbital are obtained by minimizing the energy of the lowest  $^5S^o$  state. The  $5s$  orbital was optimized on the average energy of  $2s^2 2p^3 4s^3 S^o$  and  $2s^2 2p^3 4s^5 S^o$  states. The  $3p$  orbital is used to improve the ground-state energy and accordingly its parameters are optimized on the  $2s^2 2p^4 3P^e$  state. The average energy of  $2s^2 2p^3 3p^3 P^e$  and  $2s^2 2p^3 3p^5 P^e$  states is used to optimize  $4p$  parameters with configurations  $2s^2 2p^3 4p^3 P^e$  and  $2s^2 2p^3 4p^5 P^e$ . Similarly, parameters for the  $5p$  orbital were obtained on the average energy of  $4p^3 P^e$  and  $4p^5 P^e$  states. The  $3d$  and  $4d$  orbitals are obtained on the energies of  $2s^2 2p^3 3d^3 D^o$  and  $2s^2 2p^3 4d^5 D^o$ , respectively. We have also obtained  $4f$  and  $5d$  orbitals but their effect was found to be negligible and therefore these were dropped from the final calculation. The parameters for all these orbitals are given in Table I.

These orbitals are then used to construct all the configurations to include "internal," "semixternal," and all the major "all external" correlations effects. These configurations are listed in Table II for even- and odd-

TABLE I. The values of parameters for the atomic orbitals for Ca XIII.

Orbital	Coefficient	Power of $r$	Exponent
3s	0.208 264 0	1	15.510 536
	-1.787 479 8	2	4.993 998
	2.345 276 6	3	4.965 391
4s	5.986 435 3	1	2.772 518
	-11.161 583 8	2	5.608 273
	13.662 874 4	3	5.534 040
5s	-9.720 900 7	4	5.434 630
	3.122 494 0	1	1.985 957
	-6.256 560 7	2	4.676 018
	19.088 677 1	3	4.175 824
3p	-20.046 172 4	4	4.713 858
	3.510 021 7	5	4.542 951
	0.588 052 6	2	7.925 266
	-1.167 191 3	3	4.334 604
	0.460 035 5	2	15.403 263
4p	-6.348 026 3	3	2.565 674
	6.897 549 2	4	3.122 448
	0.851 402 4	2	16.103 421
5p	-0.873 656 2	3	9.514 906
	0.695 830 4	4	4.498 314
	-0.883 632 3	5	2.481 528
	1.000 000 0	3	4.531 850
3d	0.963 228 6	3	4.299 670
4d	-1.429 483 8	4	3.106 880

parity states. The calculation performed with this complete set of configurations is labeled "CI1." We have also carried out another calculation "CI2" with a compact set of configurations in which all the configurations with  $a_{ij} < 0.005$  and a negligible contribution to the oscillator strength were discarded. This resulted in a substantial reduction of the number of configurations for each state which facilitated the intermediate-coupling calculation.

As the nuclear charge increases, the relativistic effects become more and more important. We, therefore, performed a separate calculation by including spin-dependent terms of the Breit-Pauli Hamiltonian in the nonrelativistic Hamiltonian (Glass and Hibbert [18]). The compact set of configurations used in the CI2 calculation is employed for the calculation in intermediate coupling. The terms of the Breit-Pauli Hamiltonian included are, spin-orbit (S-O), spin-other-orbit (S-O-O), spin-spin (S-S), Darwin ( $D$ ) and mass correction ( $M$ ). The wave functions are then represented by a  $J$ -dependent configuration-interaction expansion,

$$\Phi_j(J) = \sum_{i=1}^m b_{ij} \phi_i(\alpha_i L_i S_i J). \quad (3)$$

The sum over  $i$  includes all those configurations whose orbital and spin angular momenta  $L_i$  and  $S_i$  couple to give the total angular momentum

$$J = L_i + S_i. \quad (4)$$

The coupling coefficients  $a_{ij}$  and  $b_{ij}$  in Eqs. (1) and (3) are the eigenvector components of the Hamiltonian obtained by diagonalizing the respective Hamiltonian.

TABLE II. Set of configurations used for Ca XIII states.

Even parity		Odd parity	
$2s^2 2p^4$		$2snp^5$	$n = 2, 3$
$2p^6$		$2s^2 2p^3 nd$	$n = 3, 4$
$2p^4 msns$	$m, n = 3, 4$	$2s^2 2p^3 ns$	$n = 3 - 5$
$2p^5 np$	$n = 3 - 5$	$2p^5 nd$	$n = 3, 4$
$2s^2 2p^4 np$	$n = 3 - 5$	$2p^5 ns$	$n = 3, 4$
$2s^2 2p^2 3pnp$	$n = 4, 5$	$2p^4 3pns$	$n = 4, 5$
$2s 2p^4 nd$	$n = 3, 4$	$2p^4 3pnd$	$n = 4, 5$
$2s 2p^4 ns$	$n = 3 - 5$	$2s^2 2p^2 msnp$	$m = 3 - 5, n = 3, 4$
$2s^2 2p^2 nl^2$	$n = 3 - 4, l = 0 - 2$	$2s 2p^3 mdns$	$m = 3, 4, n = 4, 5$
$2s^2 2p^2 5p^2$		$2s^2 2p^2 mdnp$	$m, n = 3, 4$
$2s^2 2p^2 3snd$	$n = 3, 4$	$2s 2p^3 3ns^2$	$n = 3, 5$
$2s 2p^3 msnp$	$m, n = 3, 4$	$2s 2p^3 np^2$	$n = 3 - 5$
$2s^2 2p^2 3pnp$	$n = 4, 5$	$2s 2p^4 np$	$n = 3 - 5$

## III. RESULTS AND DISCUSSION

The energies and oscillator strengths calculated for Ca XIII in the *LS* and intermediate coupling, using the wave functions constructed as described in Sec. II, are discussed in the following.

A. *LS* Coupling

The energies of the states of Ca XIII obtained in the present two sets of nonrelativistic calculations are given in Table III along with the observed values compiled by Sugar and Corliss [19]. The observed term energies are

TABLE III. Calculated and observed *LS* energies (in a.u.) of Ca XIII states relative to the ground state.

State	Even parity			State	Odd parity		
	CI1	CI2	Observed		CI1	CI2	Observed
$2s^2 2p^4 3P^e$	0.0	0.0	0.0	$2s 2p^5 3P^o$	2.7286	2.7045	2.8876
$2s^2 2p^4 1D^e$	0.3429	0.3309	0.3501	$2s 2p^5 1P^o$	3.7744	3.7500	3.8225
$2s^2 2p^4 1S^e$	0.7157	0.7046	0.7621	$2s^2 2p^3 (4S^o) 3s 5S^o$	15.1541	15.1233	
$2p^6 1S^e$	6.3904	6.3716	6.5108	$2s^2 2p^3 (4S^o) 3s 3S^o$	15.3507	15.3254	15.3244
$2s^2 2p^3 (4S^o) 3p 5P^e$	15.8699	15.8476		$2s^2 2p^3 3s 3D^o$	15.7252	15.7017	15.6931
$2s^2 2p^3 (4S^o) 3p 3P^e$	16.0395	16.0721		$2s^2 2p^3 3s 1D^o$	15.8234	15.8123	15.7804
$2s^2 2p^3 (2D^o) 3p 1P^e$	16.3538	16.3546		$2s^2 2p^3 3s 3P^o$	15.9737	15.9751	
$2s^2 2p^3 (2D^o) 3p 3D^e$	16.3869	16.3713		$2s^2 2p^3 3s 1P^o$	16.0719	16.0773	16.0980
$2s^2 2p^3 (2D^o) 3p 3F^e$	16.4289	16.4376		$2s^2 2p^3 (4S^o) 3d 5D^o$	16.8100	16.7830	
$2s^2 2p^3 (2D^o) 3d 1F^e$	16.4592	16.4603		$2s^2 2p^3 (4S^o) 3d 3D^o$	17.0006	17.0030	16.9952
$2s^2 2p^3 3p 3S^e$	16.6227	16.6025		$2s^2 2p^3 (4S^o) 3d 1S^o$	17.3300	17.2987	
$2s^2 2p^3 (2D^o) 3p 3P^e$	16.6894	16.7228		$2s^2 2p^3 (2D^o) 3d 1P^o$	17.4372	17.4564	
$2s^2 2p^3 (2P^o) 3p 3D^e$	16.6934	16.7034		$2s^2 2p^3 (2D^o) 3d 3D^o$	17.4615	17.4587	17.4334
$2s^2 2p^3 (2P^o) 3p 1D^e$	16.7463	16.7487		$2s^2 2p^3 (2D^o) 3d 1D^o$	17.4856	17.5014	
$2s^2 2p^3 (2P^o) 3p 1P^e$	16.7573	16.7665		$2s^2 2p^3 (2D^o) 3d 3P^o$	17.5141	17.5402	17.5420
$2s^2 2p^3 (2P^o) 3p 3P^e$	16.8070	16.8307		$2s^2 2p^3 (2D^o) 3d 3S^o$	17.5658	17.5461	17.5543
$2s^2 2p^3 (2D^o) 3p 1D^e$	16.9877	16.9988		$2s^2 2p^3 (2P^o) 3d 3P^o$	17.6442	17.7623	17.6770
$2s^2 2p^3 3p 1S^e$	17.2567	17.2395		$2s^2 2p^3 (2P^o) 3d 3D^o$	17.7209	17.7368	17.7971
$2s 2p^4 3s 5P^e$	17.4791	17.4779		$2s^2 2p^3 (2P^o) 3d 1D^o$	17.7870	17.8079	17.7414
$2s 2p^4 (4P) 3s 3P^e$	17.7631	17.7621		$2s^2 2p^3 (2P^o) 3d 1P^o$	17.9724	17.9994	18.0322
$2s 2p^4 3s 3D^e$	18.4015	18.4091		$2s 2p^4 3p 5D^o$	18.2357	18.2179	
$2s 2p^4 3s 1D^e$	18.5841	18.5863		$2s 2p^4 (4P) 3p 3D^o$	18.3567	18.3276	
$2s 2p^4 3s 3S^e$	18.9223	18.9182		$2s 2p^4 3S^o$	18.3725	18.3514	
$2s 2p^4 3s 1S^e$	19.0899	19.0862		$2s 2p^4 (4P) 3d 3S^o$	18.4106	18.3940	
$2s 2p^4 (2P) 3s 3P^e$	19.1321	19.1367		$2s 2p^4 (4P) 3p 3P^o$	18.4586	18.4692	
$2s 2p^4 3s 1P^e$	19.2039	19.1905		$2s 2p^4 (2D) 3p 1P^o$	19.1153	19.1975	
$2s 2p^4 3d 5P^e$	19.2140	19.1905		$2s 2p^4 (2D) 3p 1D^o$	19.2639	19.2745	
$2s 2p^4 3d 3D^e$	19.4237	19.5672		$2s 2p^4 3p 1S^o$	19.9521	19.9477	
$2s 2p^4 3d 3S^e$	20.0698	20.0398		$2s 2p^4 (2P) 3p 3S^o$	19.9790	19.9858	
$2s 2p^4 3d 1P^e$	20.1676	20.2048		$2s^2 2p^3 4s 3S^o$	20.5791	20.5819	
				$2s^2 2p^3 4d 1S^o$	21.7400	21.7432	

tabulated relative to the  $LS$  center of gravity of the  $2s^2 2p^4 \ ^3P_J$  levels for the comparison with our calculated  $LS$  values. The energies of Ca XIII states as calculated in the CI2 calculation are very close to those obtained in the CI1 calculation as can be seen from Table III. The agreement with the observed values is reasonably good, within 0.3%, except for the  $2s^2 2p^4 \ ^1S^e$ ,  $2s^2 2p^4 \ ^1D^e$ , and  $2s 2p^5 \ ^3P^o$  states where present CI2 calculated energies differ with the observed ones by 0.058, 0.019, and 0.183, a.u., respectively, leading to a maximum difference of about 8%. It is mainly due to the choice of  $1s$ ,  $2s$ , and  $2p$

orbitals chosen for the  $2s^2 2p^4 \ ^3P^e$  ground state in the present calculations. Baluja and Zeippen (BZ) [9] have compared their excitation energies for several transitions with other theoretical works and with experimental values of Baskin and Stoner [20]. Our  $LS$  excitation energies are in good agreement with these and in fact are closer to the experimental values except for the excitation energy for the transition  $2p^6 \ ^1S^e - 2s 2p^5 \ ^1P^o$ , for which our calculated value is in disagreement with others by about 14%. However, our value for the excitation energy of this transition disagrees with the value given by Sugar

TABLE IV. The oscillator strengths for the transitions among Ca XIII states. The numbers in brackets indicate powers of 10:  $a[\pm b] \equiv a \times 10^{\pm b}$ .

Transition $i-f$	Oscillator strength			
	L(CI1)	V(CI1)	L(CI2)	BZ [9]
$2s^2 2p^4 \ ^3P^e - 2p^3 3s \ ^3S^o$	4.1787[-2]	4.1019[-2]	4.1691[-2]	
$2s^2 2p^4 \ ^3P^e - 2p^3 3d \ ^3S^o$	1.7528[-1]	1.5496[-1]	1.7657[-1]	
$2s^2 2p^4 \ ^3P^e - 2s 2p^4 3p \ ^3S^o$	4.1412[-2]	3.7831[-2]	4.3770[-2]	
$2p^3(^4S^o)3p \ ^3P^e - 2s 2p^4 3p \ ^3S^o$	1.6092[-2]	1.2935[-2]	1.2186[-2]	
$2p^3 3s \ ^3S^e - 2p^3 3p \ ^3P^e$	2.5036[-1]	2.4638[-1]	2.8110[-1]	
$2s^2 2p^4 \ ^3P^e - 2p^3 3s \ ^3D^o$	6.3385[-2]	6.1239[-2]	6.0918[-2]	
$2s^2 2p^4 \ ^3P^e - 2p^3 3d \ ^3D^o$	2.8840[-1]	2.7423[-1]	2.9629[-1]	
$2s^2 2p^4 \ ^3P^e - 2p^3(^2D^o)3d \ ^3D^o$	5.1729[-1]	4.8677[-1]	5.2596[-1]	
$2s^2 2p^4 \ ^3P^e - 2p^3(^2P^o)3e \ ^3D^o$	5.5450[-1]	5.2857[-1]	5.3947[-1]	
$2p^3(^4S^o)3p \ ^3P^e - 2p^3 3d \ ^3D^o$	1.9457[-1]	2.4469[-1]	1.9922[-1]	
$2p^3 3s \ ^3D^o - 2p^3(^4S)3p \ ^3P^e$	2.7453[-3]	3.1743[-3]	2.8564[-3]	
$2s 2p^4 \ ^3P^e - 2s 2p^5 \ ^3P^o$	1.0997[-1]	9.9808[-2]	1.1008[-1]	1.079[-1]
$2s^2 2p^4 \ ^3P^e - 2p^3 3s \ ^3P^o$	3.6415[-2]	3.7456[-2]	3.5578[-2]	
$2s^2 2p^4 \ ^3P^e - 2p^3(^2D)3d \ ^3P^o$	5.2454[-1]	4.8495[-1]	4.8887[-1]	
$2s^2 2p^4 \ ^3P^e - 2p^3(^2P)3d \ ^3P^o$	3.0277[-2]	2.6698[-2]	2.9548[-2]	
$2p^3(^4S^o)3p \ ^3P^e - 2p^3 3d \ ^3P^o$	1.7975[-2]	1.9597[-2]	1.7855[-2]	
$2p^3(^2P^o)3p \ ^3D^e - 2p^3 3s \ ^3P^o$	1.6403[-1]	1.7512[-1]	1.6466[-1]	
$2s 2p^5 \ ^3P^o - 2p^3 3p \ ^3S^e$	1.9161[-3]	8.7908[-4]	2.0933[-3]	
$2p^3 3s \ ^3P^o - 2p^3 3p \ ^3S^e$	2.7871[-2]	2.9125[-2]	2.6894[-2]	
$2s 2p^5 \ ^3P^o - 2s 2p^4 3s \ ^3S^e$	1.5507[-2]	1.6761[-2]	1.5236[-2]	
$2p^3 3s \ ^3D^o - 2p^3 3p \ ^3D^e$	8.3388[-2]	8.1818[-2]	8.5127[-2]	
$2p^3 3s \ ^3D^o - 2p^3(^2P^o)3p \ ^3D^e$	8.4608[-3]	7.7137[-3]	9.1356[-3]	
$2s^2 2p^4 \ ^1D^e - 2s 2p^5 \ ^1P^o$	1.4075[-1]	1.0441[-1]	1.3985[-1]	1.138[-1]
$2s^2 2p^4 \ ^1D^e - 2p^3 3s \ ^1P^o$	3.0290[-2]	3.2023[-2]	2.9394[-2]	
$2s^2 2p^4 \ ^1D^e - 2p^3(^2D)3d \ ^1P^o$	1.3485[-1]	1.2469[-1]		
$2s 2p^5 \ ^1P^o - 2p^6 \ ^1S^e$	1.220[-1]	8.5115[-2]	1.2135[-1]	
$2s 2p^5 \ ^1P^o - 2s^2 2p^3 3p \ ^1S^e$	2.2845[-3]	2.1908[-3]	2.3137[-3]	
$2s 2p^5 \ ^1P^o - 2s^2 2p^3 \ ^1D^e$	3.5446[-3]	2.7752[-3]	3.46214[-3]	
$2s^2 2p^3 3s \ ^1P^o - 2s^2 2p^3 3p \ ^1D^e$	9.5006[-2]	9.9016[-2]	9.6139[-2]	
$2s^2 2p^3 3s \ ^1D^o - 2s^2 2p^3 3p \ ^1P^e$	3.5595[-2]	3.8698[-2]	3.5608[-2]	
$2s^2 2p^3 3p \ ^1P^e - 2s^2 2p^3 3d \ ^1D^o$	1.0657[-1]	1.1992[-1]	1.0578[-1]	
$2s^2 2p^4 \ ^1D^e - 2p^3 3s \ ^1D^o$	1.0115[-1]	9.8737[-2]	9.6989[-2]	
$2s^2 2p^4 \ ^1D^e - 2p^3 3d \ ^1D^o$	1.4130[-1]	1.2559[-1]	1.4399[-1]	
$2p^3 3s \ ^1P^o - 2p^3(^2D)3p \ ^1P^e$	6.4806[-3]	7.6983[-3]	6.5433[-3]	
$2p^3 3d \ ^1P^o - 2p^3(^2D)3p \ ^1P^e$	3.4828[-2]	3.9567[-2]	3.5142[-2]	
$2s^2 2p^4 \ ^1S^e - 2s 2p^5 \ ^1P^o$	6.2142[-2]	8.8902[-2]	6.3428[-2]	6.41[-2]
$2s^2 2p^4 \ ^1S^e - 2s^2 2p^3 3s \ ^1P^o$	1.4164[-1]	1.3426[-1]	1.3306[-1]	
$2s^2 2p^4 \ ^1S^e - 2s^2 2p^3 3d \ ^1P^o$	1.7293[-1]	1.5678[-1]	1.7145[-1]	
$2p^3 3s \ ^5S^o - 2p^3 3p \ ^5P^e$	2.9207[-1]	2.8546[-1]	2.9628[-1]	
$2p^3 3p \ ^5P^e - 2s 2p^4 3p \ ^5S^o$	1.8533[-2]	1.2398[-2]	1.8638[-2]	
$2p^3 3p \ ^5P^e - 2p^3 3d \ ^5D^o$	2.1071[-1]	3.1872[-1]	2.1022[-1]	
$2p^3 3p \ ^5P^e - 2s 2p^4 3p \ ^5D^o$	7.0632[-2]	6.7185[-2]	7.3481[-2]	
$2p^3 3p \ ^5P^e - 2s^2 2p^3 4d \ ^5D^o$	3.4020[-1]	3.0389[-1]		
$2s 2p^4 3s \ ^5P^e - 2s 2p^4 3p \ ^5D^o$	2.0908[-1]	1.9140[-1]	2.1009[-1]	

and Corliss [19] only by 2.5% (0.067 a.u.).

Table IV contains the oscillator strengths for dipole transitions among the states of O I-like calcium ion as calculated in the present two *LS*-coupling calculations. We have included only the length value of the oscillator strength obtained in our CI2 calculation. These are compared with the values obtained by Baluja and Zeippen [9] in their *LS*-coupling calculation. They reported the oscillator strength between the states of  $n=2$  complex and used  $3s$ ,  $3p$ , and  $3d$  correlation orbitals to account for the electron correlations. They used the experimental energies instead of theoretical ones.

The close agreement between the length  $L$  and velocity  $V$  forms of the oscillator strengths is a necessary (but of course not sufficient) condition for the good quality wave functions. The length form emphasizes the asymptotic part of the wave function whereas the velocity form weights the intermediate region. For most of the transitions reported here, we get a very good agreement between these values. Our length values, which are supposed to be more accurate, are in remarkably good agreement with those obtained by Fawcett [10] and Baluja and Zeippen [9]. Both of these authors used experimental values for the excitation energies. The values reported by

Cheng, Kim, and Desclaux [8] are higher than all other values. This is mainly due to neglect of the electron-correlation effects in their calculation. We will discuss the calculations of Cheng, Kim, and Desclaux [8] and Fawcett [10] in more detail in the intermediate-coupling section.

The  $f$  values reported here between the *LS* terms are obtained through a step-by-step improvement of wave functions. We have tried to include all the important configuration-interaction effects and therefore have reasons to believe that the  $f$  values reported here provide an improvement over the values reported so far and can be used with confidence in the astrophysical applications.

### B. Intermediate coupling

The results in the intermediate coupling are obtained by including one- and two-electron operators of the Breit-Pauli Hamiltonian in the nonrelativistic Hamiltonian. The spin-forbidden transitions which are not allowed in the *LS* coupling become allowed through the inclusion of the spin-dependent operators of the Breit-Pauli Hamiltonian. Different *LS* terms of the same parity couple to give the same value of  $J$ . It is, therefore, important that

TABLE V. Fine-structure energy levels of Ca XIII relative to the ground-level energy (in a.u.).

Level	Calculated	Observed	Level	Calculated	Observed
Even parity			Odd parity		
$2s^2 2p^4 \ ^3P_2^e$	0.0	0.0	$2s^2 2p^3(2P^e)3s \ ^3P_2^o$	16.1154	
$2s^2 2p^4 \ ^3P_1^e$	0.1095	0.1145	$2s^2 2p^3(2P^e)3s \ ^1P_1^o$	16.2024	
$2s^2 2p^4 \ ^3P_0^e$	0.1286	0.1316	$2s^2 2p^3(2D^e)3s \ ^1P_1^o$	16.2225	16.1502
$2s^2 2p^4 \ ^1D_2^e$	0.4050	0.4019	$2s^2 2p^3(4S^e)3d \ ^5D_0^o$	16.8886	
$2s^2 2p^4 \ ^1S_0^e$	0.7949	0.8138	$2s^2 2p^3(4S^e)3d \ ^5D_1^o$	16.8883	
$2p^6 \ ^1S_0^e$	6.6896	6.5626	$2s^2 2p^3(4S^e)3d \ ^5D_2^o$	16.8875	
$2s^2 2p^3(4S^e)3p \ ^5P_3^e$	15.9326		$2s^2 2p^3(4S^e)3d \ ^5D_3^o$	16.8865	
$2s^2 2p^3(4S^e)3p \ ^5P_2^e$	15.9230		$2s^2 2p^3(4S^e)3d \ ^5D_4^o$	16.8781	
$2s^2 2p^3(4S^e)3p \ ^5P_1^e$	15.9135		$2s^2 2p^3(4S^e)3d \ ^3D_1^o$	17.1252	
$2s^2 2p^3(4S^e)3p \ ^3P_2^e$	16.1853		$2s^2 2p^3(4S^e)3d \ ^3D_2^o$	17.1143	17.0362
$2s^2 2p^3(4S^e)3p \ ^3P_1^e$	16.1708		$2s^2 2p^3(4S^e)3d \ ^3D_3^o$	17.1289	17.0541
$2s^2 2p^3(4S^e)3p \ ^3P_0^e$	16.1906		$2s^2 2p^3(2D^e)3d \ ^1S_0^o$	17.3953	
$2s^2 2p^3(2D^e)3p \ ^3D_2^e$	16.4464		$2s^2 2p^3(2D^e)3d \ ^3F_3^o$	17.3983	
$2s^2 2p^3(2D^e)3p \ ^3D_1^e$	16.4039		$2s^2 2p^3(2D^e)3d \ ^3F_2^o$	17.4095	
$2s^2 2p^3(2D^e)3p \ ^1P_1^e$	16.4903		$2s^2 2p^3(2D^e)3d \ ^3G_3^o$	17.4461	
$2s^2 2p^3(2D^e)3p \ ^3F_3^e$	16.5124		$2s^2 2p^3(2D^e)3d \ ^3G_4^o$	17.4519	
$2s^2 2p^3(2D^e)3p \ ^3F_2^e$	16.5029		$2s^2 2p^3(2D^e)3d \ ^3G_2^o$	17.4461	
$2s^2 2p^3(2P^e)3p \ ^3D_3^e$	16.7981		$2s^2 2p^3(2D^e)3d \ ^1G_4^o$	17.4789	
Odd parity			$2s^2 2p^3(2D^e)3d \ ^3D_1^o$	17.5386	17.4422
$2s^2 2p^5 \ ^3P_2^o$	2.8478	2.8170	$2s^2 2p^3(2D^e)3d \ ^3D_2^o$	17.5802	17.4870
$2s^2 2p^5 \ ^3P_1^o$	2.9380	2.9080	$2s^2 2p^3(2D^e)3d \ ^3D_3^o$	17.5897	17.5012
$2s^2 2p^5 \ ^3P_0^o$	2.9912	2.9621	$2s^2 2p^3(2D^e)3d \ ^3P_2^o$	17.6598	17.5461
$2s^2 2p^5 \ ^1P_1^o$	3.9503	3.8743	$2s^2 2p^3(2D^e)3d \ ^3P_1^o$	17.6649	17.5510
$2s^2 2p^3(4S^o)3s \ ^5S_2^o$	15.1806		$2s^2 2p^3(2P^e)3d \ ^1F_3^o$	17.6785	
$2s^2 2p^3(4S^o)3s \ ^3S_1^o$	15.3873	15.3760	$2s^2 2p^3(2D^e)3d \ ^3P_0^o$	17.6831	
$2s^2 2p^3(2D^e)3s \ ^3D_1^o$	15.7487	15.7321	$2s^2 2p^3(2D^e)3d \ ^1D_2^o$	17.6497	17.5461
$2s^2 2p^3(2D^e)3s \ ^3D_2^o$	15.7519	15.7342	$2s^2 2p^3(2D^e)3d \ ^1F_3^o$	17.7368	
$2s^2 2p^3(2D^e)3s \ ^3D_3^o$	15.7713	15.7570	$2s^2 2p^3(2P^e)3d \ ^3F_4^o$	17.7600	
$2s^2 2p^3(2D^e)3s \ ^1D_2^o$	15.8818	15.8312	$2s^2 2p^3 3d \ ^3P_0^o$	17.9212	
$2s^2 2p^3(2P^e)3s \ ^3P_0^o$	16.0662		$2s^2 2p^4 3p \ ^5D_4^o$	18.3932	
$2s^2 2p^3(2P^e)3s \ ^3P_1^o$	16.0785		$2s^2 2p^4 3p \ ^5D_0^o$	18.4279	

TABLE VI. The oscillator strengths for the transitions among Ca XIII fine-structure levels. The numbers in squared brackets refer to the numbers in the reference list. The numbers in brackets indicate powers of 10:  $\alpha[\pm b] \equiv \alpha \times 10^{\pm b}$ .

Transition	Oscillator Strength					
	<i>i-f</i>	L	V	HFR [10]	SS [3]	MCDF [8]
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^3 S_1^o$		4.4074[-2]	4.5300[-2]	5.520[-2]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 S_1^o$		3.4895[-2]	3.4984[-2]	4.400[-2]		
$2s^2 2p^4 3P_0^e - 2s^2 2p^3 3s^3 S_1^o$		4.0848[-2]	4.0149[-2]	4.901[-2]		
$2p^3 3s^3 S_0^o - 2s^2 2p^3 3p^3 P_1^e$		9.8264[-2]	1.1201[-1]			
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^5 S_2^o$		5.1428[-4]	5.2431[-4]			
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^5 S_2^o$		1.0710[-4]	1.0808[-4]			
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^3 D_3^o$		4.8491[-2]	4.9174[-2]	5.780[-2]		
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^3 D_2^o$		2.0743[-2]	2.1229[-2]	2.420[-2]		
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^3 D_1^o$		8.5226[-4]	8.6304[-4]			
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 D_2^o$		2.6739[-2]	2.6185[-2]	3.030[-2]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 D_1^o$		2.3912[-2]	2.3767[-2]	2.661[-2]		
$2s^2 2p^4 3P_0^e - 2s^2 2p^3 3s^3 D_1^o$		3.9335[-2]	3.8006[-2]	4.200[-2]		
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3d^3 D_2^o$		5.1498[-2]	4.8758[-2]			
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3d^3 D_3^o$		2.5425[-1]	2.3812[-1]	2.586[-1]		
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^1 D_2^o$		4.8690[-3]	5.2722[-3]	5.600[-3]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^1 D_2^o$		6.3896[-3]	5.4230[-3]	7.300[-3]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3d^1 S_0^o$		3.0118[-4]	2.6020[-4]			
$2s^2 2p^4 3P_2^e - 2s^2 2p^5 3P_2^o$		8.3931[-2]	6.7777[-2]	8.440[-2]	9.218[-2]	9.220[-2]
$2s^2 2p^4 3P_2^e - 2s^2 2p^5 3P_1^o$		3.0553[-2]	2.3199[-2]	3.040[-2]	3.303[-2]	3.323[-2]
$2s^2 2p^4 3P_1^e - 2s^2 2p^5 3P_2^o$		4.5846[-2]	3.8723[-2]	4.930[-2]	5.060[-2]	5.045[-2]
$2s^2 2p^4 3P_1^e - 2s^2 2p^5 4P_0^o$		3.907[-2]	3.003[-2]	3.900[-2]	4.290[-2]	4.285[-2]
$2s^2 2p^4 3P_0^e - 2s^2 2p^5 3P_1^o$		1.0962[-1]	8.8312[-2]	1.120[-1]	1.213[-1]	1.210[-1]
$2s^2 2p^4 3P_1^e - 2s^2 2p^5 3P_1^o$		2.8416[-2]	2.2208[-2]	2.860[-2]	3.124[-2]	3.128[-2]
$2s^2 2p^4 3P_2^e - 2s^2 2p^3 3s^3 P_2^o$		1.2184[-2]	1.2381[-2]			
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 P_2^o$		2.7642[-2]	2.8159[-2]	3.23[-2]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 P_1^o$		4.4341[-3]	4.5546[-3]	4.800[-3]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 P_0^o$		7.1692[-3]	7.4349[-3]	8.000[-3]		
$2s^2 2p^4 3P_1^e - 2s^2 2p^3 3s^3 P_0^o$		1.2015[-2]	1.2366[-2]	1.330[-2]		
$2s^2 2p^4 3P_0^e - 2s^2 2p^3 3s^3 P_1^o$		5.8739[-2]	5.9680[-2]			
$2s^2 2p^5 3P_0^o - 2s^2 2p^3 3p^3 P_1^e$		2.7593[-4]	2.9368[-4]			
$2s^2 2p^3 3s^3 P_0^o - 2s^2 2p^3 3p^3 P_1^e$		2.6647[-4]	2.9292[-4]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^5 3P_2^o$		2.6433[-3]	2.6984[-3]		2.223[-3]	2.383[-3]
$2s^2 2p^4 1D_2^e - 2s^2 2p^5 3P_1^o$		3.5714[-5]	1.2807[-5]		3.000[-5]	4.988[-5]
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^5 S_2^o$		6.5254[-8]	4.2271[-8]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 D_2^o$		3.8919[-4]	4.4849[-4]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 P_2^o$		1.4088[-2]	1.3321[-2]	1.500[-2]		
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 P_1^o$		2.6043[-3]	2.8663[-3]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^1 D_2^o$		7.6096[-2]	7.7907[-2]	1.012[-1]		
$2s^2 2p^5 3P_0^o - 2p^6 1S_0^e$		8.8834[-4]	8.7698[-4]			9.089[-4]
$2s^2 2p^5 1P_1^o - 2p^6 1S_0^e$		1.2538[-1]	8.0308[-2]	1.230[-2]		1.443[-2]
$2s^2 2p^4 3P_2^e - 2s^2 2p^5 1P_1^o$		3.7528[-3]	2.2029[-3]		3.07[-3]	3.438[-3]
$2s^2 2p^4 3P_1^e - 2s^2 2p^5 1P_1^o$		2.4062[-4]	1.1822[-4]		1.900[-4]	2.131[-4]
$2s^2 2p^4 3P_0^e - 2s^2 2p^5 1P_1^o$		1.7381[-3]	2.4899[-3]		1.350[-3]	1.519[-3]
$2s^2 2p^4 1D_2^e - 2s^2 2p^5 1P_1^o$		1.4079[-1]	9.4427[-2]	1.420[-1]	1.543[-1]	1.542[-1]
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 S_1^o$		4.4429[-4]	4.0529[-4]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 D_1^o$		8.7796[-4]	1.0168[-3]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 D_3^o$		1.9658[-3]	1.7435[-3]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3s^3 D_1^o$		8.7796[-4]	1.0168[-3]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3d^5 D_2^o$		1.8512[-6]	1.4319[-6]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3 3d^5 D_3^o$		9.1360[-6]	8.9071[-6]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3(^4S)3d^2 D_3^o$		1.0784[-3]	9.7110[-4]			
$2s^2 2p^4 1D_2^e - 2s^2 2p^3(^4S)3d^2 D_3^o$		2.3703[-3]	2.2417[-3]			
$2s^2 2p^4 3P_1^o - 2s^2 2p^3(^2D)3d^3 P_0^o$		1.0486[-1]	9.5091[-2]			
$2s^2 2p^4 3P_1^e - 2s^2 2p^3(^2P)3d^3 P_0^o$		7.6142[-2]	6.7160[-2]			
$2p^3 3p^3 P_1^e - 2s^2 2p^3 3d^1 S_0^o$		5.4718[-4]	5.0242[-4]			
$2s^2 2p^4 1S_0^e - 2s^2 2p^5 3P_1^o$		2.9191[-3]	2.5776[-3]		2.460[-3]	2.622[-3]
$2s^2 2p^4 1S_0^e - 2s^2 2p^5 1P_1^o$		6.5748[-2]	9.9001[-2]	7.300[-2]	7.160[-2]	7.149[-2]
$2s^2 2p^4 1S_0^e - 2s^2 2p^3 3s^1 P_1^o$		1.3339[-1]	1.2203[-1]			

TABLE VI. (Continued).

Transition <i>i-f</i>	Oscillator Strength				
	L	V	HFR [10]	SS [3]	MCDF [8]
$2s^2 2p^4 \ ^1S_0^e - 2s^2 2p^3 3s \ ^3D_1^o$	8.7936[-4]	7.1438[-4]			
$2s^2 2p^3 3s \ ^3S_2^o - 2s^2 2p^3 3p \ ^3P_2^e$	9.9538[-2]	9.3898[-2]			
$2s^2 2p^3 3s \ ^3S_2^o - 2s^2 2p^3 3p \ ^3P_1^e$	5.9212[-2]	5.6578[-2]			
$2s^2 2p^3 3s \ ^5S_2^o - 2s^2 2p^3 3p \ ^3P_2^e$	3.2415[-3]	3.2329[-3]			
$2s^2 2p^3 3s \ ^4S_2^o - 2s^2 2p^3 3p \ ^3P_1^e$	3.9914[-4]	4.0218[-4]			
$2s^2 2p^3 3s \ ^3D_2^o - 2s^2 2p^3 3p \ ^5P_2^e$	9.5615[-6]	1.2260[-5]			
$2s^2 2p^3 3s \ ^3D_2^o - 2s^2 2p^3 3p \ ^5P_1^e$	1.1161[-6]	9.8770[-5]			
$2s^2 2p^3 3p \ ^5P_1^e - 2s^2 2p^3 3d \ ^5D_0^o$	4.3875[-2]	6.3595[-2]			
$2s^2 2p^3 3p \ ^3P_2^e - 2s^2 2p^3 3d \ ^5D_3^o$	1.2215[-1]	1.7649[-1]			
$2s^2 2p^3 3p \ ^5P_2^e - 2s^2 2p^3 3d \ ^3D_3^o$	8.7997[-4]	9.6855[-4]			
$2s^2 2p^4 \ ^3P_1^e - 2s^2 2p^3 3d \ ^5D_0^o$	4.6640[-4]	4.1507[-4]			
$2s^2 2p^4 \ ^3P_2^e - 2s^2 2p^3 3d \ ^5D_2^o$	1.2051[-3]	1.1196[-3]			
$2s^2 2p^4 \ ^3P_2^e - 2s^2 2p^3 3d \ ^5D_3^o$	2.8211[-4]	2.7333[-4]			
$2s^2 2p^4 \ ^3P_2^e - 2s^2 2p^4 \ (^2D) 3d \ ^3F_3^o$	1.4744[-2]	1.3845[-2]	2.180[-2]		
$2s^2 2p^4 \ ^3P_2^e - 2s^2 2p^3 3d \ ^3G_3^o$	2.8862[-3]	2.7086[-3]			
$2s^2 2p^4 \ ^1D_2^e - 2s^2 2p^3 3d \ ^3F_3^o$	9.9402[-4]	9.6055[-4]			
$2s^2 2p^4 \ ^1D_2^e - 2s^2 2p^3 3d \ ^3G_3^o$	4.9947[-3]	4.7991[-3]	5.800[-3]		
$2s^2 2p^4 3s \ ^5P^e - 2s^2 2p^4 3p \ ^5D^o$	2.1330[-1]	1.8636[-1]			

all the states which mix with the ones considered for the transition are represented by accurate configuration-interaction wave functions.

The energies of the fine-structure levels and the oscillator strengths between these levels are given in Tables V and VI, respectively. The fine-structure-level energies presented here are in very good agreement with the observed values tabulated by Sugar and Corliss [19]. The maximum difference is about 2.3%. In general, the length and velocity values are in good agreement, within 10%, except for some transitions for which these differ by as much as a factor of 2. This is due to the use of the common set of orbitals for all the states and perhaps inadequate all-external correlation effects considered here. The present fine-structure oscillator strengths are compared where available with the line strengths reported by Cheng, Kim, and Desclaux [8] who used the MCDF technique with only  $n=2$  configurations, superstructure (SS) results of Mason [3], and relativistic Hartree-Fock calculated values of Fawcett [10]. All these calculations account for the relativistic effects. As can be seen from Table VI, our length values of the fine-structure oscillator strengths agree remarkably with those of Fawcett [10] for the transitions between  $n=2$  levels. The  $f$  values reported by Cheng, Kim, and Desclaux and Mason [3] are slightly higher than ours, which seems to be due to insufficient configuration interaction in their calculation. Fawcett [10] also reports  $f$  values for the transitions between the fine-structure levels of  $n=2$  configurations and  $3s$  and  $3d$  excited-state configurations. It is to be noticed that his values are consistently larger than values reported in the present calculation. It could be due to the fact that he did not explicitly include enough electron-correlation effects for these states. We have used extensive configuration interaction and our length and velocity values for these transitions are in excellent agreement. We, therefore, believe that our results

for these transitions are better than the ones reported by Fawcett.

Consider, for example, the  $2s^2 2p^4 \ ^3P_2 - 2s^2 2p^3 3s \ ^3S_1^o$  transition. The present length and velocity values are 4.4074[-2] and 4.5300[-2], respectively, and the Hartree-Fock relativistic value reported by Fawcett [10] is 5.52[-2], showing a difference of about 20%. Similarly, for transitions  $2s^2 2p^4 \ ^3P_1 - 2s^2 2p^3 3s \ ^3S_1^o$  and  $2s^2 2p^4 \ ^1D_2 - 2s^2 2p^3 3s \ ^1D_2^o$  his results are higher by more than 28% and 33%, respectively. For most transitions, however, the discrepancy between the two sets of results is below 15%.

Included in the above table are also the  $f$  values for the intercombination transitions which are of special interest for the calculation of the chemical abundances due to their small values. The emission lines pertaining to the allowed transitions are often highly saturated, making them useless for the abundance studies. Some of the oscillator strengths reported here for the intercombination transitions have not been considered in earlier calculations. It is seen that for such spin-changing transitions, the inclusion of two-electron operators, S-S and S-O-O, of the Breit-Pauli Hamiltonian in the calculation reduces the oscillator strengths by about 11% to 50%. Table VII compares these values obtained with and without the inclusion of these terms in the Hamiltonian for some of the transitions. Also tabulated are the transition probabilities ( $A_L$ ) for these transitions. The length form of the oscillator strength for the transition  $2s^2 2p^4 \ ^3P_2 \rightarrow 2s^2 2p^3 3s \ ^5S_2^o$  increases by about 12% as a result of neglecting spin-spin and spin-other-orbit terms, whereas the value for the transitions  $2s^2 2p^4 \ ^1D_2 \rightarrow 2s^2 2p^3 3s \ ^3P_1^o$  gets overestimated by almost a factor of 2. These operators have negligible effect on the  $f$  values for the spin-allowed dipole transitions. It is to be noted that the inclusion of these terms in the calculation is very

TABLE VII. Effect of S-S and S-O-O Breit-Pauli terms on the intercombination transition oscillator strengths. Numbers in brackets indicate powers of 10:  $\alpha[\pm b] \equiv \alpha \times 10^{\pm b}$ .

Transition <i>i-f</i>	With S-S, S-O-O			Without S-S, S-O-O	
	$f_L$	$f_V$	$A_L$ (sec <sup>-1</sup> )	$f_L$	$f_V$
$2s^2 2p^4 \ ^3P_2^e - 2s^2 2p^3 3s \ ^5S_2^o$	5.1428[-4]	5.2431[-4]	3.8277[9]	5.7436[-4]	5.7590[-4]
$2s^2 2p^4 \ ^3P_1^e - 2s^2 2p^3 3s \ ^5S_2^o$	1.0710[-4]	1.0808[-4]	4.6895[8]	1.3444[-4]	1.3510[-4]
$2s^2 2p^3 3p \ ^5P_2^e - 2s^2 2p^3 3d \ ^3D_3^o$	7.1926[-4]	7.9424[-4]	2.4002[7]	8.7997[-4]	9.6855[-4]
$2s^2 2p^4 \ ^3P_2^e - 2s^2 2p^3 3d \ ^5D_3^o$	2.8211[-4]	2.7333[-4]	1.8462[9]	3.4748[-4]	3.3699[-4]
$2s^2 2p^4 \ ^1D_2^e - 2s^2 2p^3 3s \ ^3S_1^o$	3.3847[-4]	3.1031[-4]	4.0685[9]	3.4256[-4]	4.0353[-4]
$2s^2 2p^4 \ ^1D_2^e - 2s^2 2p^3 3s \ ^3P_1^o$	1.7434[-3]	1.9159[-3]	2.2935[10]	2.5982[-3]	2.8594[-3]
$2s^2 2p^4 \ ^1D_2^e - 2s^2 2p^3 3s \ ^3P_2^o$	1.4088[-2]	1.3321[-2]	1.1159[11]	1.5536[-2]	1.4958[-2]
$2s^2 2p^4 \ ^1D_2^e - 2s^2 2p^3 3d \ ^3F_3^o$	7.4979[-4]	7.2361[-4]	4.9691[9]	9.9402[-4]	9.6055[-4]

time consuming and therefore expensive. However, we feel that for the calculation of oscillator strengths for the intercombination transitions in the Breit-Pauli approximation, it is important to include these terms in the Hamiltonian.

#### IV. CONCLUSION

We have used extensive configuration-interaction wave functions to calculate oscillator strengths for the transitions between *LS* states and fine-structure levels belonging to the  $n=2$  and  $n=3$  complex. The energies obtained in the present calculation agree fairly well with the observed values. Our length values of the oscillator strengths for the transitions between  $n=2$  levels are in very good agreement with the values reported by Fawcett while values of Cheng, Kim, and Desclaux [8] and Mason [3] are higher for the lack of sufficient electron correlations in their calculations. For the transition between  $n=2$  and  $n=3$  levels, our values show an improvement over the ones obtained by Fawcett. There is good agreement between our results obtained in length and velocity

forms. The present results are tested using a more elaborate configuration set and it is found that results do not change by more than 10%. It is also seen that neglecting spin-spin and spin-other-orbit terms of the Breit-Pauli Hamiltonian overestimates the values of the oscillator strengths of intercombination transitions considerably, varying from 12% to about 50%. These two-electron operator terms, therefore, should be taken into account while calculating oscillator strengths for the intercombination transitions in the Breit-Pauli approximation. We expect our results to be of high accuracy and therefore confidently recommend their use in any application.

#### ACKNOWLEDGMENTS

We would like to thank Dr. D. S. Leckrone for his interest in this work and for useful discussions. One of us (K. S. B.) would like to thank National Research Council of the National Academy of Science for support. This work was funded by NASA Grant No. NASA-RTOP-188-38-53-14.

- [1] H. E. Saraph, M. J. Seaton, and J. Shemming, *Philos. Trans. R. Soc.* **264**, 77 (1969).
- [2] A. K. Pradhan, *J. Phys.* **B 7**, L503 (1974).
- [3] H. E. Mason, *Mon. Not. R. Astron. Soc.* **170**, 651 (1974).
- [4] A. K. Bhatia, U. Feldman, and G. A. Doschek, *Astron. Astrophys.* **80**, 22 (1980); *J. Appl. Phys.* **51**, 1464 (1980).
- [5] K. Butler and C. Mendoza, *Mon. Not. R. Astron. Soc.* **208**, 17p (1984).
- [6] K. J. Reed and R. J. W. Henry, *Phys. Rev. A* **40**, 1823 (1989).
- [7] R. D. Cowan, Los Alamos Scientific Laboratory Report No. LA-6679-MS, 1979 (unpublished).
- [8] K. T. Cheng, Y. K. Kim, and J. P. Desclaux, *At. Data Nucl. Data Tables* **24**, 111 (1979).
- [9] K. L. Baluja and C. J. Zeippen, *J. Phys.* **B 21**, 15 (1988).
- [10] B. C. Fawcett, *At. Data Nucl. Data Tables* **34**, 215 (1986).
- [11] S. S. Tayal and R. J. W. Henry, *Phys. Rev. A* **39**, 4531 (1989).
- [12] A. Hibbert, E. Biemont, M. Godefroid, and N. Vaeck, *J. Phys.* **B 24**, 3983 (1991).
- [13] A. Hibbert, *Comput. Phys. Commun.* **9**, 141 (1975).
- [14] W. Eissner and H. Nussbaumer, *J. Phys.* **B 2**, 1028 (1969).
- [15] J. P. Desclaux, *Comput. Phys. Commun.* **9**, 31 (1975).
- [16] R. D. Cowan, *J. Opt. Soc. Am.* **58**, 808 (1968); *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981); R. D. Cowan and D. C. Griffin, *J. Opt. Soc. Am.* **66**, 1010 (1976).
- [17] E. Clementi and C. Roetti, *At. Data Nucl. Data Tables* **14**, 177 (1974).
- [18] R. Glass and A. Hibbert, *Comput. Phys. Commun.* **16**, 19 (1978).
- [19] J. Sugar and C. Corliss, *J. Phys. Chem. Ref. Data* **14**, Suppl. 2 (1985).
- [20] S. Baskin and J. O. Stoner, *Atomic Energy-Level and Gortian Diagrams* (North-Holland, Amsterdam, 1978), Vol. II.