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Atomic data from the IRON Project

XXXIII. Radiative rates for the intercombination transitions in the carbon isoelectronic sequence⋆

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Abstract. Radiative decay rates are computed with the atomic structure code SUPERSTRUCTURE for the $2s2p^3\ {}^5S^o_2 - 2s^22p^2\ {}^3P_1$, $^3P_2$ and $^1D_2$ intercombination transitions of the carbon isoelectronic sequence ($6 \leq Z \leq 28$). Contributions from configuration interaction and relativistic corrections are carefully studied, in particular the spin–spin interaction that is shown to be of considerable importance for low Z. By extensive comparisons with other theoretical datasets and measurements of the $^5S^o_2$ radiative lifetime and the $B = A(^5S^o_2 - {}^3P_2)/A(^5S^o_2 - {}^3P_1)$ branching ratio, we are able to assign accuracy ratings to the present transition probabilities. The transitions to the ground term are believed to be accurate to better than 10% whereas the smaller A-values belonging to transitions to the $^1D_2$ are not expected to be accurate to more than 20%.

Key words: atomic data

1. Introduction

Intercombination transitions are observed in the spectra of a wide variety of astronomical bodies where they may be used as plasma diagnostics to estimate the electron density, temperature and chemical abundances. In this context, the intercombination transitions involving the $2s2p^3\ {}^5S^o_2$ metastable level in ions of the carbon isoelectronic sequence, in particular those down to the $2s^22p^2\ {}^3P_{1,2}$ ground term, are among the most interesting in laboratory astrophysics. Their complex properties present an opportunity to test the state of the art in observation, theory and experiment. For instance, by making use of a systematic configuration interaction method (SCIV3), Brage et al. (1997) and Fleming & Brage (1997) have recently reported that in N II and O III the branching ratio

$$B = \frac{A(^5S^o_2 - {}^3P_2)}{A(^5S^o_2 - {}^3P_1)} \quad (1)$$

shows a reduction of approximately 20% from the expected value of ~ 3 for low Z (Ellis & Martinson 1984), which Fleming & Brage have attributed in the case of

Table 1. Configuration bases used in approximations A, B, C and D

Approx. A	Approx. B	Approx. C	Approx. D
$2s^22p^2$	$2s^22p^2$	$2s^22p^2$	$2s^22p^2$
$2s2p^3$	$2s2p^3$	$2s2p^3$	$2s2p^3$
$2p^4$	$2p^4$	$2p^4$	$2p^4$
$2s^22p3l$	$2s^22p3l$	$2s^22p3l$	$2s^22p3l$
$2s2p^23l$	$2s2p^23l$	$2s2p^23l$	$2s2p^23l$
$2p^33l$	$2p^33l$	$2p^33l$	$2p^33l$
$2s^23l3l'$	$2s^23l3l'$	$2s^23l3l'$	$2s^23l3l'$
$2s2p3l3l'$	$2s2p3l3l'$	$2s2p3l3l'$	$2s2p3l3l'$
$2p^23l3l'$	$2p^23l3l'$	$2p^23l3l'$	$2p^23l3l'$
	$2s^22p4l$	$2s^22p4l$	$2s^22p4l$
	$2s2p^24l$	$2s2p^24l$	$2s2p^24l$
	$2p^34l$	$2p^34l$	$2p^34l$
		$2s^24l4l'$	$2s^24l4l'$
		$2s2p4l4l'$	$2s2p4l4l'$
		$2p^24l4l'$	$2p^24l4l'$
			$2s^23l4l'$
			$2s2p3l4l'$
			$2p^23l4l'$

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⋆ A detailed table of the present transition probabilities is available in electronic form from the CDS via anonymous ftp 130.79.128.5 or via http://cdsweb.u-strasbg.fr/Abstract.html

Table 2. Scaling parameters λ_{nl} used to generate the orbitals for the four approximations (A, B, C and D) as a function of nuclear charge number Z. The negative scaling parameters denote Coulombic correlation orbitals

Approx.	Z	1s	2s	2p	$\bar{3}$s	$\bar{3}$p	$\bar{3}$d	$\bar{4}$s	$\bar{4}$p	$\bar{4}$d	$\bar{4}$f
A	6	1.4845	1.2005	1.1931	−0.6857	−0.6700	−0.8232				
	7	1.4816	1.2134	1.1889	−0.8802	−0.8355	−0.9790				
	8	1.4790	1.2233	1.1877	−0.9690	−0.9488	−1.0869				
	9	1.4768	1.2305	1.1874	−1.0268	−1.0324	−1.1672				
	10	1.4750	1.2359	1.1876	−1.0713	−1.0975	−1.2296				
	11	1.4735	1.2401	1.1880	−1.1067	−1.1499	−1.2796				
	12	1.4715	1.2434	1.1885	−1.1360	−1.1927	−1.3207				
	13	1.4712	1.2461	1.1890	−1.1605	−1.2285	−1.3549				
	14	1.4701	1.2484	1.1895	−1.1813	−1.2588	−1.3840				
	15	1.4694	1.2502	1.1900	−1.1991	−1.2847	−1.4091				
	16	1.4687	1.2518	1.1905	−1.2147	−1.3073	−1.4309				
	17	1.4676	1.2533	1.1910	−1.2281	−1.3271	−1.4501				
	18	1.4675	1.2544	1.1914	−1.2404	−1.3446	−1.4670				
	19	1.4670	1.2555	1.1918	−1.2512	−1.3601	−1.4819				
	20	1.4640	1.2565	1.1922	−1.2610	−1.3740	−1.4954				
	21	1.4661	1.2574	1.1925	−1.2696	−1.3865	−1.5076				
	22	1.4657	1.2581	1.1929	−1.2776	−1.3979	−1.5187				
	23	1.4653	1.2588	1.1932	−1.2849	−1.4082	−1.5287				
	24	1.4650	1.2594	1.1935	−1.2915	−1.4176	−1.5378				
	25	1.4648	1.2600	1.1938	−1.2976	−1.4262	−1.5463				
	26	1.4644	1.2606	1.1941	−1.3030	−1.4342	−1.5541				
	27	1.4642	1.2610	1.1943	−1.3083	−1.4415	−1.5612				
	28	1.4639	1.2615	1.1946	−1.3131	−1.4483	−1.5678				
B	6	1.4876	1.3629	1.4477	−0.9568	−0.9034	−0.8980	−0.9801	−0.9038	−0.8054	−1.4310
	7	1.4859	1.2164	1.3672	−0.9726	−0.9681	−1.0450	−1.2391	−1.3474	−1.1014	−1.6560
	8	1.4829	1.1703	1.3167	−0.9874	−1.0151	−1.0008	−1.2848	−1.4717	−1.3811	−1.8184
	9	1.4806	1.1759	1.2372	−1.0327	−1.0588	−1.1839	−1.4140	−1.4784	−2.5867	−1.9320
	10	1.4791	1.1784	1.0910	−1.0607	−1.0179	−1.2418	−1.5346	−1.4712	−2.5018	−2.0172
C	6	1.4880	1.3743	1.4501	−0.9358	−0.9051	−0.9033	−0.9862	−0.9137	−1.2442	−1.7041
	7	1.4858	1.2233	1.3688	−0.8774	−0.8708	−0.9337	−1.3839	−1.4446	−1.3558	−1.9491
	8	1.4828	1.1728	1.3165	−0.9992	−1.0014	−1.0348	−1.4466	−1.5128	−1.4705	−2.1028
	9	1.4806	1.1758	1.2376	−1.0301	−1.0547	−1.1796	−1.5190	−1.5218	−1.6381	−2.1918
	10	1.4790	1.1784	1.0924	−1.0562	−1.0120	−1.2395	−1.5661	−1.5140	−1.7519	−2.2709
D	6	1.4900	1.2135	1.2247	−1.0021	−0.9410	−1.0509	−1.2043	−1.1210	−1.3507	−1.6188
	7	1.4859	1.2165	1.2922	−0.9663	−0.9390	−1.0226	−1.2516	−1.3748	−1.5689	−1.7879
	8	1.4830	1.1807	1.2948	−0.9845	−1.0032	−1.1025	−1.3003	−1.4583	−1.7073	−1.9380

O III to the contribution from the relativistic two-body Breit interaction. This is an important conclusion because the Breit formulation although assumed correct has not been fully verified by experiment. Since B is a measurable quantity and the departure from the first-order value is large, an experimental benchmark would be invaluable. A recent measurement of the 2143/2139 Å emission doublet from N II in a low-pressure inductively coupled plasma by Curry et al. (1997) resulted in a value for B of 2.27 ± 0.23, somewhat lower than obtained by the SCIV3 method of Brage et al. (1997), but in agreement within the experimental errors. Moreover, the former compare their results with the discordant values by Musielok et al. (1996) and Bridges et al. (1996) obtained in an atmospheric pressure wall-stabilised arc discharge ($B = 2.24 \pm 0.06$ and $B = 2.45 \pm 0.04$, respectively). Following a discussion of the experimental difficulties, Curry et al. favour their low-pressure source and a higher resolution (compared to other experiments) as it permits to reduce line-broadening and unfold weak blends. The situation is similar for the

Table 3. A-values (s^{-1}) for the $^5S^o_2 - {}^3P_1$ transition in the carbon sequence computed in approximations A, A′, B, C and D. $a \pm b \equiv a \times 10^{\pm b}$

Z	A	A′	B	C	D
6	8.85+0	8.35+0	7.81+0	8.41+0	8.99+0
7	5.14+1	4.84+1	5.44+1	5.24+1	5.50+1
8	2.27+2	2.15+2	2.36+2	2.34+2	2.38+2
9	7.99+2	7.61+2	8.24+2	8.13+2	
10	2.36+3	2.25+3	2.38+3	2.35+3	
11	6.10+3	5.86+3			
12	1.43+4	1.38+4			
13	3.10+4	2.99+4			
14	6.32+4	6.12+4			
15	1.23+5	1.19+5			
16	2.29+5	2.23+5			
17	4.14+5				
18	7.28+5				
19	1.25+6				
20	2.11+6	2.07+6			
21	3.51+6				
22	5.76+6				
23	9.31+6				
24	1.49+7				
25	2.35+7				
26	3.67+7	3.61+7			
27	5.67+7				
28	8.64+7				

radiative lifetimes of the $^5S^o_2$ level along the sequence. In the case of N II and O III, there is excellent agreement (better than 1%) between the theoretical estimates by Brage et al. (1997) and Fleming & Brage (1997) and the values that have emerged from the ion-trap experiments (Calamai & Johnson 1991; Johnson et al. 1984, 1991), which contrasts with the wide scatter (as large as a factor of 2) found in previous calculations. However, a recent and very accurate (∼0.5%) measurement by Träbert et al. (1998) for N II in a heavy-ion storage ring results in a significantly higher value thus leaving the pursuit of the benchmark still open.

The emission from N II($^5S^o_2$) is an important feature in the Earth's aurora and dayglow (Torr & Torr 1985; Siskind & Barth 1987; Bucsela & Sharp 1989) where the level is populated by photodissociative ionization of N_2 (Dalgarno et al. 1981; Victor & Dalgarno 1982). From the observed doublet Bucsela & Sharp have obtained a value of $B = 1.72 \pm 0.24$ which is significantly lower than both the latest laboratory and theoretical estimates. The O III doublet at 1666/1600 Å is frequently observed in astronomical sources of low to medium density, and in some conditions the branching ratio is found to depend on optical depth (Kastner & Bhatia 1989). Furthermore, in the

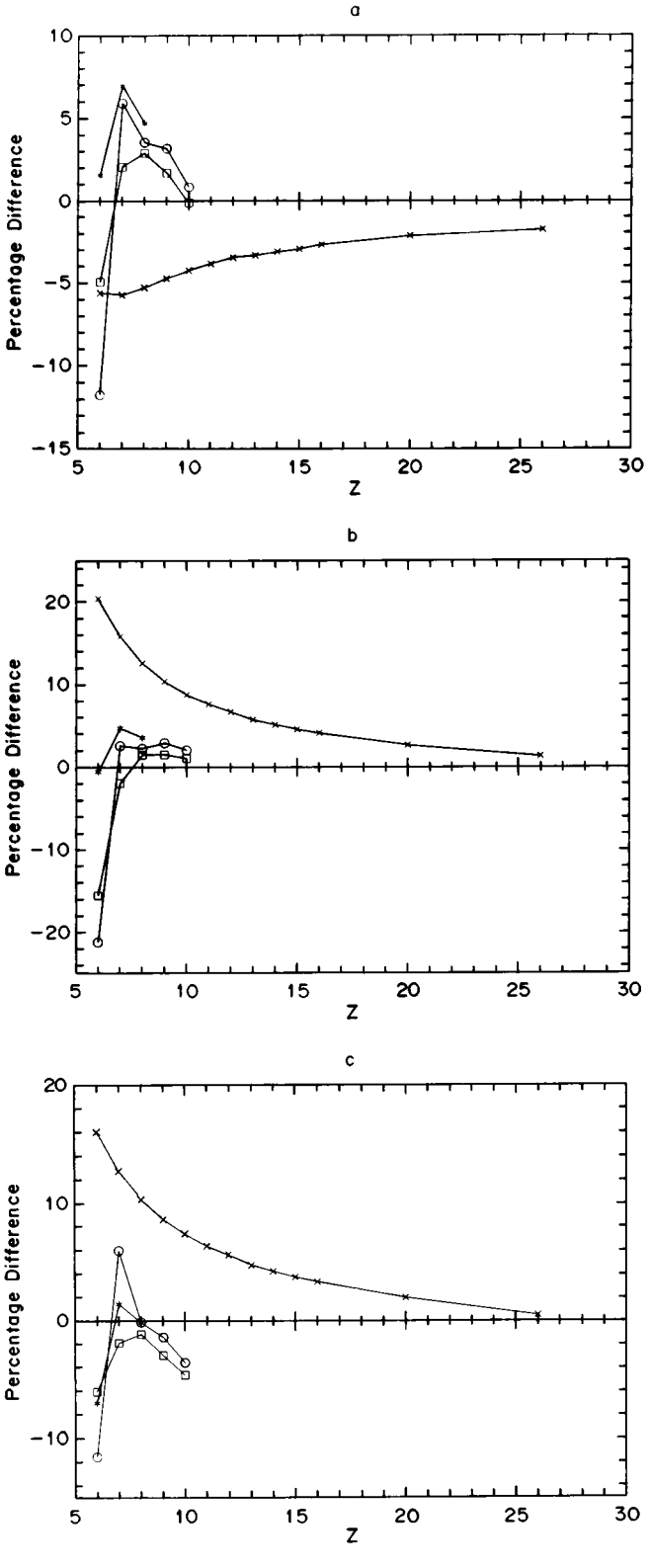

Fig. 1. Percentage difference of A-values computed in approximations A′ (x), B (circles), C (squares) and D (asterisk) with respect to the standard approximation A. **a)** $^5S^o_2 - {}^3P_1$. **b)** $^5S^o_2 - {}^3P_2$. **c)** $^5S^o_2 - {}^1D_2$

Table 4. A-values (s^{-1}) for the $^5S^o_2 - {}^3P_2$ transition in the carbon sequence computed in approximations A, A′, B, C and D. $a \pm b \equiv a \times 10^{\pm b}$

Z	A	A′	B	C	D
6	2.07+1	2.49+1	1.63+1	1.75+1	2.06+1
7	1.24+2	1.44+2	1.27+2	1.22+2	1.30+2
8	5.62+2	6.32+2	5.74+2	5.70+2	5.82+2
9	2.00+3	2.20+3	2.06+3	2.03+3	
10	5.90+3	6.41+3	6.02+3	5.96+3	
11	1.51+4	1.63+4			
12	3.49+4	3.72+4			
13	7.38+4	7.80+4			
14	1.46+5	1.53+5			
15	2.71+5	2.84+5			
16	4.82+5	5.02+5			
17	8.22+5				
18	1.35+6				
19	2.17+6				
20	3.37+6	3.46+6			
21	5.13+6				
22	7.64+6				
23	1.12+7				
24	1.61+7				
25	2.29+7				
26	3.23+7	3.27+7			
27	4.49+7				
28	6.21+7				

Table 5. A-values (s^{-1}) for the $^5S^o_2 - {}^1D_2$ transition in the carbon sequence computed in approximations A, A′, B, C and D. $a \pm b \equiv a \times 10^{\pm b}$

Z	A	A′	B	C	D
6	2.52−5	2.93−5	2.23−5	2.37−5	2.35−5
7	4.85−4	5.46−4	5.14−4	4.75−4	4.92−4
8	6.37−3	7.03−3	6.36−3	6.29−3	6.36−3
9	5.67−2	6.16−2	5.59−2	5.51−2	
10	3.76−1	4.03−1	3.62−1	3.58−1	
11	1.98+0	2.11+0			
12	8.79+0	9.26+0			
13	3.39+1	3.55+1			
14	1.16+2	1.21+2			
15	3.65+2	3.78+2			
16	1.05+3	1.09+3			
17	2.83+3				
18	7.15+3				
19	1.70+4				
20	3.82+4	3.89+4			
21	8.10+4				
22	1.62+5				
23	3.07+5				
24	5.47+5				
25	9.18+5				
26	1.45+6	1.46+6			
27	2.17+6				
28	3.06+6				

case of symbiotic stars the observed O III intercombination ratios are noticeably higher than the theoretical value; this unusual effect has been interpreted by Kastner et al. (1989) as the result of Bowen pumping. The corresponding lines in Fe XXI (271/242 Å) were first identified in the EUV spectra of solar flares by Dere (1978) although any conclusion about the magnitude of B, which is expected to be close to unity, is spoilt by the blending with a strong line of Fe XIV.

Previous datasets for the intercombination transitions of the carbon sequence have been computed by Cheng et al. (MCDF, 1985) in a Multiconfiguration Dirac-Fock approach; by Froese Fischer & Saha (MCHF, 1985) in the well established Breit-Pauli Multiconfiguration Hartree-Fock method; by Bhatia (1982), Bhatia et al. (1987), Bhatia & Kastner (1993), Bhatia & Doschek (1993a, 1993b, 1993c, 1995) and Mason & Bhatia (1978) (to be hereafter referred to as SSTR) using the atomic structure code SUPERSTRUCTURE by Eissner et al. (1974); and by Aggarwal (1986), Aggarwal et al. (1997a, 1997b) and Bell et al. (1995) (referred to as CIV3) with the CIV3 program of Hibbert (1975). Comparisons and assessments of these datasets have yet to be made in order to determine much needed accuracy ratings.

In the on-going IRON Project (IP, Hummer et al. 1993), we are interested in computing atomic data, namely radiative and collisional rates, in isoelectronic sequences for astrophysical plasma diagnostics. Although the emphasis is on the iron-group elements due to the needs of recent space missions, e.g. the Solar and Heliospheric Observatory (SOHO), good accord with the available detailed calculations for the lower members (C, N and O say) is always a requisite in order to ensure good representations of electron correlation effects and relativistic couplings at higher Z. Electron impact excitation data involving the $^5S^o_2$ level in ions of the carbon sequence have been reported within the IP by Lennon & Burke (1994). We are concerned here with the corresponding radiative rates, and in the context of the current discussion of radiative lifetimes and branching ratios, we are interested in studying isoelectronic trends in particular those of the Breit operators. We attempt to end up also with a ranked radiative dataset more accurate than previous work and one that will be included in the IP public databases. Note that a complete list of papers in the IP series can be found at the URL http://www.am.qub.ac.uk/projects/iron/papers/papers.html. In Sect. 2 we describe the present computational

Table 6. Radiative lifetimes (ms) for the $^5S^o_2$ metastable state of the carbon sequence resulting from approximations A, A′, B, C and D. $a \pm b \equiv a \times 10^{\pm b}$

Z	A	A′	B	C	D
6	3.38+1	3.01+1	4.15+1	3.86+1	3.38+1
7	5.70+0	5.21+0	5.51+0	5.75+0	5.41+0
8	1.27+0	1.18+0	1.23+0	1.24+0	1.22+0
9	3.58−1	3.37−1	3.47−1	3.52−1	
10	1.21−1	1.15−1	1.19−1	1.20−1	
11	4.71−2	4.51−2			
12	2.03−2	1.96−2			
13	9.54−3	9.26−3			
14	4.79−3	4.67−3			
15	2.54−3	2.48−3			
16	1.40−3	1.38−3			
17	8.07−4				
18	4.79−4				
19	2.91−4				
20	1.81−4	1.80−4			
21	1.15−4				
22	7.38−5				
23	4.81−5				
24	3.17−5				
25	2.11−5				
26	1.42−5	1.42−5			
27	9.63−6				
28	6.60−6				

Table 7. Branching ratio $B = A(^5S^o_2 - {}^3P_2)/A(^5S^o_2 - {}^3P_1)$ in the carbon sequence obtained from approximations A, A′, B, C and D

Z	A	A′	B	C	D
6	2.34	2.98	2.09	2.08	2.29
7	2.41	2.96	2.34	2.32	2.36
8	2.47	2.94	2.44	2.44	2.44
9	2.50	2.90	2.49	2.49	
10	2.50	2.84	2.53	2.53	
11	2.48	2.78			
12	2.44	2.70			
13	2.38	2.61			
14	2.31	2.50			
15	2.21	2.38			
16	2.11	2.25			
17	1.99				
18	1.86				
19	1.73				
20	1.59	1.67			
21	1.46				
22	1.33				
23	1.20				
24	1.08				
25	0.97				
26	0.88	0.91			
27	0.79				
28	0.72				

method and in Sect. 3 results are discussed in the light of extensive comparisons. Conclusions are summarised in Sect. 4.

2. Method

The calculations of transition probabilities have been carried out with the computer program SUPERSTRUCTURE, originally developed by Eissner et al. (1974) and later modified by Nussbaumer & Storey (1978) to ensure greater flexibility in the radial functions. The method has been described in previous IP reports (Galavís et al. 1997, 1998). As discussed by Eissner (1991) the LS terms are represented by CI wavefunctions of the type

$$\Psi = \sum_i \phi_i c_i \ , \tag{2}$$

where the configuration basis functions ϕ_i are constructed from one-electron orbitals generated in two types of potentials $V(\lambda_{nl})$: the spectroscopic orbitals $P(nl)$ are calculated in a statistical Thomas–Fermi–Dirac model potential (Eissner & Nussbaumer 1969) whereas the correlation orbitals $P(\bar{n}l)$ are obtained in a Coulomb potential (Nussbaumer & Storey 1978). With regards to configuration bases, four approximations are considered as shown in Table 1. Approximation A is our main standard framework containing only configurations with $n \leq 3$ orbitals. The representations for the lower members of the sequence are progressively refined with approximations B, C and D which include configurations with $n = 4$ orbitals of increasing complexity. The adopted variational procedure minimises with equal weights the sum of energies of all the terms in specific configurations, that is

$$\mathcal{F} = \sum_{i=1}^{N} E(S_i, L_i) \ . \tag{3}$$

The 1s, 2s and 2p orbitals are chosen to minimise the sum of energies of the three terms in the $2s^22p^2$ ground configuration. The $\bar{3}$s, $\bar{3}$p and $\bar{3}$d correlation orbitals are subsequently chosen to minimise the sum of the energies of the twelve terms of the $n = 2$ complex. Finally, the $\bar{4}$s, $\bar{4}$p, $\bar{4}$d and $\bar{4}$f correlation orbitals in approximations B, C and D are optimised on the sum of the energies of the three terms within the ground configuration. The final scaling parameters are listed in Table 2.

Table 8. Comparison of the best present A-values (s^{-1}) for the $^5S^o_2 - {}^3P_1$ transition in the carbon sequence with other theoretical results. MCHF: Froese Fischer & Saha (1985). SSTR: Bhatia (1982), Bhatia et al. (1987), Bhatia & Kastner (1993), Bhatia & Doschek (1993a, 1993b, 1993c, 1995) and Mason & Bhatia (1978). MCDF: Cheng et al. (1979). CIV3: Aggarwal (1986) and Aggarwal et al. (1997a, 1997b)). SCIV3: Brage et al. (1997) and Fleming & Brage (1997). NS: Nussbaumer & Storey (1981). HB: Hibbert & Bates (1981). $a \pm b \equiv a \times 10^{\pm b}$

Z	Pres.	MCHF	SSTR	MCDF	CIV3	SCIV3	NS	HB
6	8.99+0	6.56+0						
7	5.50+1	4.05+1				5.36+1		4.8+1
8	2.38+2	1.98+2	1.45+2	1.20+2	1.67+2	2.37+2	2.12+2	
9	7.99+2	7.24+2		5.10+2				
10	2.36+3	2.18+3	1.80+3	1.66+3	1.94+3			
11	6.10+3	5.71+3		4.58+3				
12	1.43+4	1.36+4	1.18+4	1.12+4	1.23+4			
13	3.10+4	2.96+4		2.51+4				
14	6.32+4	6.07+4	5.48+4	5.25+4	6.65+4			
15	1.23+5	1.18+5		1.04+5				
16	2.29+5	2.21+5	2.07+5	1.97+5				
17	4.14+5	4.00+5		3.62+5				
18	7.28+5	7.03+5	6.63+5	6.43+5				
19	1.25+6	1.21+6		1.12+6				
20	2.11+6	2.04+6	1.95+6	1.90+6	1.88+6			
21	3.51+6	3.39+6		3.18+6				
22	5.76+6	5.56+6	5.34+6	5.25+6				
23	9.31+6	8.99+6		8.53+6				
24	1.49+7	1.44+7		1.37+7				
25	2.35+7	2.28+7	2.17+7	2.17+7				
26	3.67+7	3.56+7	3.42+7	3.40+7	3.30+7			
27	5.67+7	5.50+7		5.26+7				
28	8.64+7	8.40+7		8.02+7				

In SUPERSTRUCTURE the Hamiltonian is taken to be of the form

$$H = H_{\rm nr} + H_{\rm rc} \quad (4)$$

where $H_{\rm nr}$ is the usual non-relativistic Hamiltonian. The relativistic corrections $H_{\rm rc}$ are taken into account through the Breit-Pauli (BP) approximation (Jones 1970, 1971)

$$H_{\rm rc} = \sum_{i=1}^{N}[f_i({\rm mass}) + f_i({\rm d}) + f_i({\rm so})] + \sum_{i>j}[g_{ij}({\rm so}+{\rm so}') + g_{ij}({\rm ss}')] \quad (5)$$

where the one-body terms f_i(mass), f_i(d) and f_i(so) correspond respectively to the mass-variation correction, the Darwin term and the spin–orbit interaction; the two-body Breit terms $g_{ij}({\rm so}+{\rm so}')$ and $g_{ij}({\rm ss}')$ are the spin–other-orbit plus mutual spin–orbit and spin–spin interactions. In the present calculations, the spin–spin interaction, when included, is fully taken into account for the first three configurations in Table 1, i.e. the spectroscopic configurations. To estimate the spin–spin contribution for all configurations in the largest basis set considered here would be very costly, if not impossible. Fortunately, small-scale tests showed that the numbers reported here are not affected by more than a few % at low Z by this approximation. When Z increases, this effect decreases rapidly.

Table 9. Comparison of the best present A-values (s^{-1}) for the $^5S^o_2 - {}^3P_2$ transition in the carbon sequence with other theoretical results. Reference keys as in Table 8. $a \pm b \equiv a \times 10^{\pm b}$

Z	Pres.	MCHF	SSTR	MCDF	CIV3	SCIV3	NS	HB
6	2.06+1	1.59+1						
7	1.30+2	1.00+2				1.31+2		1.07+2
8	5.82+2	5.00+2	4.26+2	4.21+2	4.15+2	5.89+2	5.22+2	
9	2.00+3	1.84+3		1.54+3				
10	5.90+3	5.55+3	5.12+3	4.76+3	4.88+3			
11	1.51+4	1.44+4		1.27+4				
12	3.49+4	3.36+4	3.21+4	3.01+4	3.01+4			
13	7.38+4	7.14+4		6.52+4				
14	1.46+5	1.42+5	1.38+5	1.31+5	1.54+5			
15	2.71+5	2.65+5		2.48+5				
16	4.82+5	4.72+5	4.73+5	4.46+5				
17	8.22+5	8.07+5		7.68+5				
18	1.35+6	1.33+6	1.33+6	1.28+6				
19	2.17+6	2.13+6		2.06+6				
20	3.37+6	3.33+6	3.36+6	3.22+6	3.06+6			
21	5.13+6	5.07+6		4.92+6				
22	7.64+6	7.58+6	7.68+6	7.38+6				
23	1.12+7	1.12+7		1.09+7				
24	1.61+7	1.62+7		1.57+7				
25	2.29+7	2.31+7	2.31+7	2.25+7				
26	3.23+7	3.27+7	3.31+7	3.18+7	3.05+7			
27	4.49+7	4.59+7		4.45+7				
28	6.21+7	6.37+7		6.18+7				

Two-body non fine-structure terms are currently neglected in SUPERSTRUCTURE.

From perturbation theory, the relativistic wavefunction $\psi_i^{\rm r}$ can be expanded in terms of the non-relativistic functions $\psi_j^{\rm nr}$:

$$\psi_i^{\rm r} = \psi_i^{\rm nr} + \sum_{j\neq i}\psi_j^{\rm nr} \times \frac{< \psi_j^{\rm nr}|H_{\rm bp}|\psi_i^{\rm nr} >}{E_i^{\rm nr} - E_j^{\rm nr}} + \ldots \quad (6)$$

This expansion demonstrates the importance of accurate term energy separations when constructing the relativistic wave functions $\psi_i^{\rm r}$. Using accurate experimental level energies (Edlén 1985), $H_{\rm nr}$ is adjusted in order to obtain term energies (calculated from the weighted fine-structure level energies) which match experiment. This semi-empirical term energy correction (TEC) procedure was originally implemented in SUPERSTRUCTURE by Zeippen et al. (1977). Galavís et al. (1997, 1998) have shown that, in the treatment of the forbidden transitions in the carbon and oxygen sequences and of the intercombination transitions in the boron sequence, the inclusion of TECs can lead to a high degree of accuracy with a much reduced configuration basis than in a comparable purely ab initio treatment. This previous experience led to the choice of our standard representation (approximation A). Of course, the validity of this semi-empirical procedure must be checked in the case under consideration here.

Table 10. Comparison of the best present A-values (s^{-1}) for the $^5S^o_2 - {}^1D_2$ transition in the carbon sequence with other theoretical results. Reference keys as in Table 8. $a \pm b \equiv a \times 10^{\pm b}$

Z	Pres.	MCHF	SSTR	MCDF	CIV3
6	2.35−5	7.37−5			
7	4.92−4	7.25−4			
8	6.36−3	3.90−3		2.30−3	9.21−4
9	5.67−2	2.72−2		2.62−2	
10	3.76−1	2.23−1	1.97−1	2.03−1	1.15−1
11	1.98+0	1.31+0		1.19+0	
12	8.79+0	6.34+0	5.54+0	5.70+0	4.60+0
13	3.39+1	2.58+1		2.33+1	
14	1.16+2	9.26+1	8.16+1	8.41+1	9.54+1
15	3.65+2	2.96+2		2.73+2	
16	1.05+3	8.61+2		8.14+2	
17	2.83+3	2.32+3		2.25+3	
18	7.15+3	5.81+3		5.79+3	
19	1.70+4	1.36+4		1.40+4	
20	3.82+4	2.99+4	3.08+4	3.19+4	2.69+4
21	8.10+4	6.13+4		6.84+4	
22	1.62+5	1.18+5		1.38+5	
23	3.07+5	2.14+5		2.61+5	
24	5.47+5	3.62+5		4.65+5	
25	9.18+5	5.75+5	7.54+5	7.78+5	
26	1.45+6	8.55+5	1.20+6	1.22+6	1.09+6
27	2.17+6	1.19+6		1.81+6	
28	3.06+6	1.56+6		2.51+6	

The radiative rate for an electric dipole ($E1$) transition is given by the expression

$$A_{ij}(E1) = 2.6774\ 10^9 (E_i - E_j)^3 \frac{1}{g_i} S_{ij}^{E1} \qquad (s^{-1}) \ , \qquad (7)$$

where g_i is the statistical weight of the upper initial level i and energies E are expressed in Rydbergs. It is clear that the accuracy of the calculated A-values depends primarily on the quality of the wavefunctions used in evaluating the line strengths S_{ij}^{E1}, but even relatively small errors in the energy differences $(E_i - E_j)$ can reduce it because of the exponent 3 in (7). Therefore, the transition probabilities are computed with an accurate and consistent dataset of experimental energy levels (Edlén 1985).

3. Results

The transition probabilities obtained from approximations A, A′, B, C and D are tabulated in Tables 3–5. Approximation A′ is the same as A but excludes the spin–spin contribution. In Fig. 1 we compare the differences of each approximation from the standard approximation A. It may be appreciated that the neglect of the spin–spin interaction (approximation A′) leads to effects that

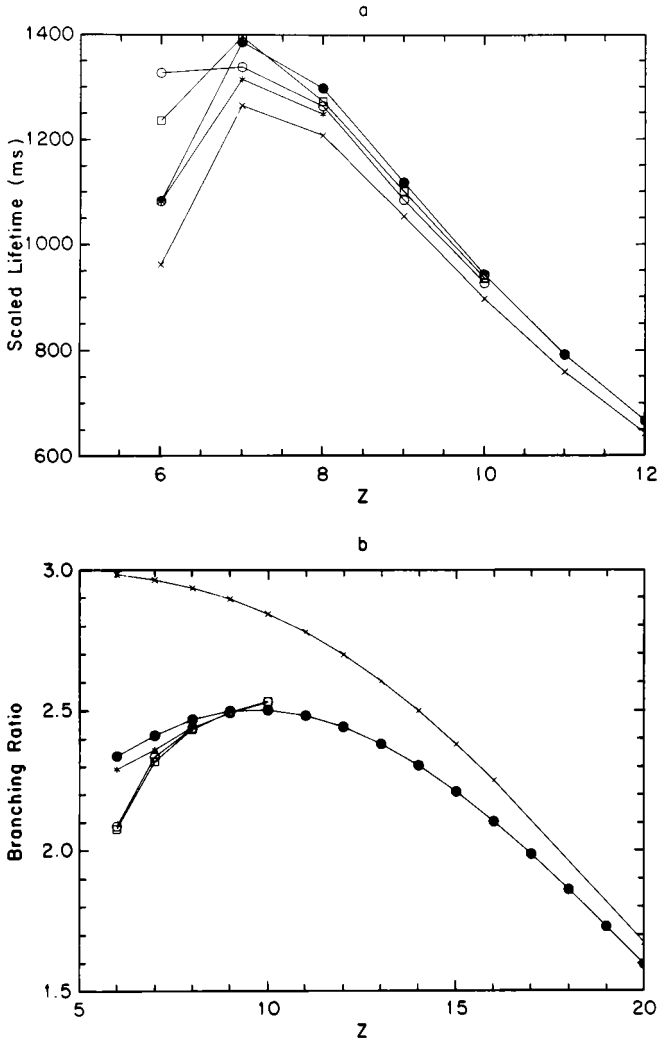

Fig. 2. Comparison of **a)** scaled $^5S^o_2$ radiative lifetimes (ms) and **b)** the branching ratios B for the different approximations considered. Filled circle: approximation A. x: A′. Circle: B. Square: C. Asterisk: D. The scaled (τ') and unscaled (τ) radiative lifetimes are related by $\tau' = \tau(Z - 4.0)^5$

decrease with Z. This finding clearly illustrates the conclusions reached by Jones (1970) regarding the character of the relativistic corrections. Namely, since the one-body and two-body (Breit) relativistic corrections respectively scale as $\alpha^2(Z - S)^4$ and $\alpha^2(Z - S)^3$, where α is the fine-structure constant and S is a screening constant, the Breit contribution decreases in importance as Z increases along the sequence. Although in the present study the spin–spin contribution increases $A(^5S^o_2 - {}^3P_1)$ by only ∼5% at low Z (see Fig. 1a), the reductions in $A(^5S^o_2 - {}^3P_2)$ and $A(^5S^o_2 - {}^1D_2)$ can be seen (Fig. 1b and Fig. 1c) to be as large as 20%. Therefore we conclude that the Breit interaction must be explicitly taken into account in the calculation of accurate radiative rates for these intercombination transitions.

Regarding electron correlation effects, it is shown in Fig. 1 that the contributions from configurations

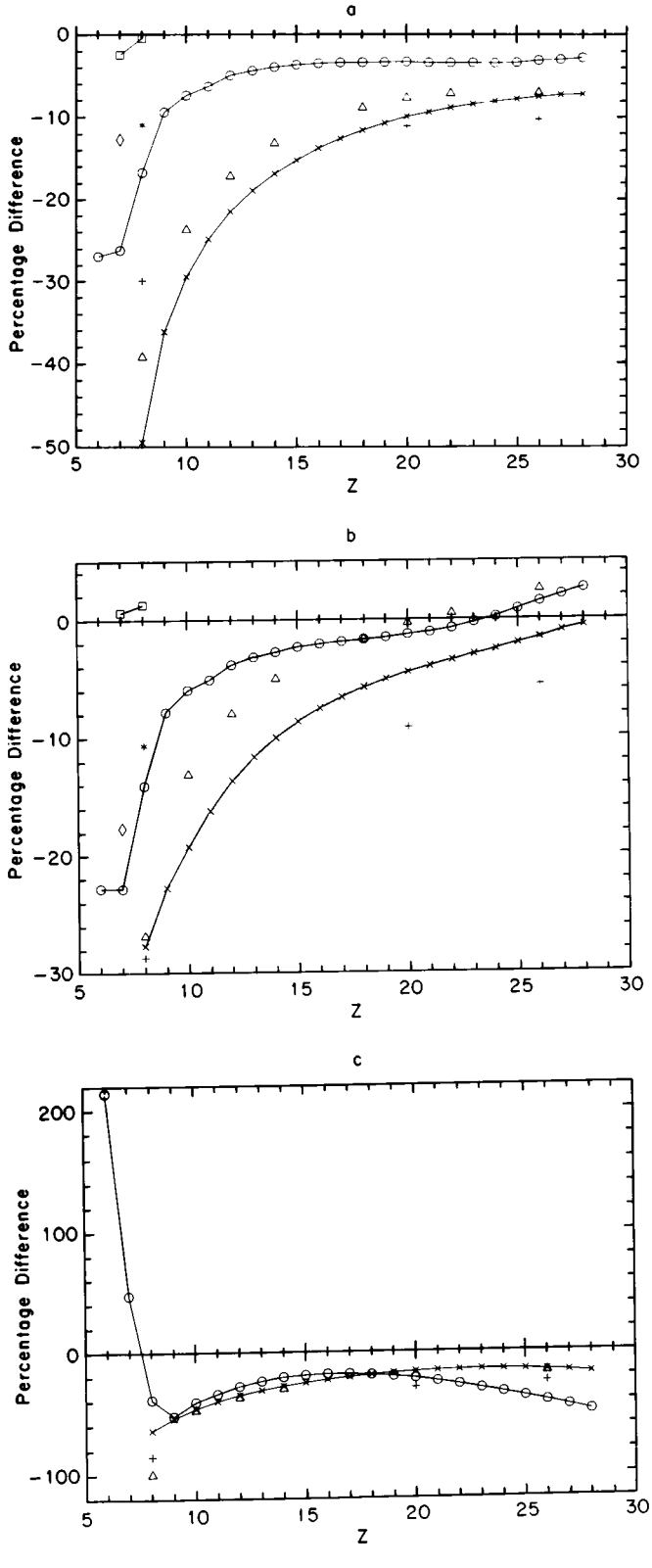

Fig. 3. Percentage difference of other theoretical A-values with respect to the best present results (approximation D). **a)** $^5S^o_2 - {}^3P_1$ **b)** $^5S^o_2 - {}^3P_2$. **c)** $^5S^o_2 - {}^1D_2$ Circle: MCHF. Triangle: SSTR. x: MCDF. Cross: CIV3. Square: SCIV3. Asterisk: Nussbaumer & Storey (1981). Rhombus: Hibbert & Bates (1981)

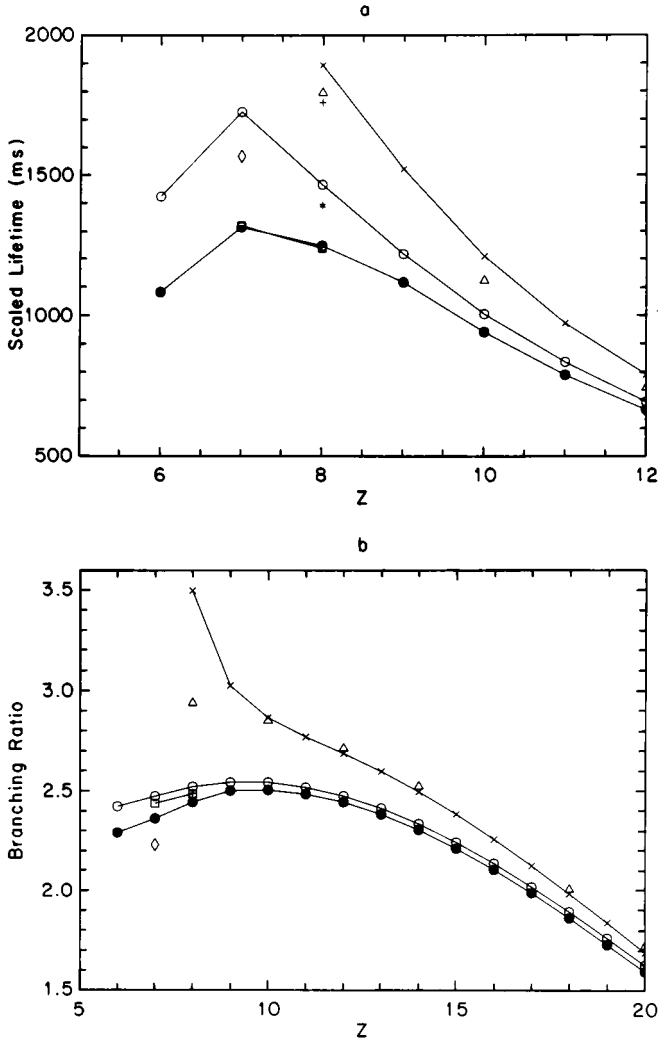

Fig. 4. Comparison of the best present **a)** scaled $^5S^o_2$ radiative lifetimes (ms) and **b)** branching ratio B with other theoretical results. Filled circle: present work. Circle: MCHF. Triangle: SSTR. x: MCDF. Cross: CIV3. Square: SCIV3. Asterisk: Nussbaumer & Storey (1981). Rhombus: Hibbert & Bates (1981). The scaled (τ') and unscaled (τ) radiative lifetimes are related by $\tau' = \tau\ (Z - 4.0)^5$

containing $n = 4$ orbitals are only conspicuous for $Z < 10$ and are very difficult to harness for the neutral ($Z = 6$). By examining the differences resulting from approximations B, C and D at low Z, it is shown in Fig. 1 that the progressive increase of the configuration basis does not necessarily lead to increasingly accurate results. It is therefore essential to include the complete complex (i.e. approximation D). From the present study it is possible to select a "best" set of data which is believed to be stable to within 5%: approximation D for $Z \leq 8$ and approximation A for $Z > 8$.

In Tables 6–7 we tabulate the $^5S^o_2$ radiative lifetimes and the B branching ratio as functions of Z for the different approximations. They are also compared in Fig. 2. In the case of lifetimes, it is seen that the exclusion of the

Table 11. Comparison of the best present radiative lifetimes (ms) for the $^5S^o_2$ state with other theoretical and experimental results. Keys for theoretical results: MCHF, Froese Fischer & Saha (1985); SSTR, Bhatia (1982), Bhatia et al. (1987), Bhatia & Kastner (1993), Bhatia & Doschek (1993a,b,c 1995) and Mason & Bhatia (1978); MCDF, Cheng et al. (1979); CIV3, Aggarwal (1986), Aggarwal et al. (1997a,b) and Bell et al. (1995); SCIV3, Brage et al. (1997) and Fleming & Brage (1997). Keys for measurements: TWP, Träbert et al. (1998); CJ, Calamai & Johnson (1991); JSKP, Johnson et al. (1991); K, Knight (1982). The experimental error is given by the quantity in brackets. $a \pm b \equiv a \times 10^{\pm b}$

	Theory								Experiment			
Z	Pres.	MCHF	SSTR	MCDF	CIV3	SCIV3	NS	HB	TWP	CJ	JSKP	K
6	3.38+1	4.45+1										
7	5.41+0	7.11+0			6.45+0	5.43+0		6.45+0	5.88(3)	5.4(3)	5.7(6)	4.2(6)
8	1.22+0	1.43+0	1.75+0	1.85+0	1.72+0	1.21+0	1.36+0				1.22(8)	
9	3.58−1	3.90−1		4.87−1								
10	1.21−1	1.29−1	1.44−1	1.56−1	1.47−1							
11	4.71−2	4.98−2		5.79−2								
12	2.03−2	2.12−2	2.28−2	2.42−2	2.36−2							
13	9.54−3	9.89−3		1.11−2								
14	4.79−3	4.94−3	5.18−3	5.45−3	4.54−3							
15	2.54−3	2.61−3		2.84−3								
16	1.40−3	1.44−3	1.47−3	1.55−3								
17	8.07−4	8.28−4		8.84−4								
18	4.79−4	4.90−4	5.01−4	5.19−4								
19	2.91−4	2.98−4		3.14−4								
20	1.81−4	1.85−4	1.87−4	1.94−4	2.01−4							
21	1.15−4	1.17−4		1.22−4								
22	7.38−5	7.54−5	7.68−5	7.84−5								
23	4.81−5	4.91−5		5.09−5								
24	3.17−5	3.24−5		3.35−5								
25	2.11−5	2.15−5	2.20−5	2.23−5								
26	1.42−5	1.45−5	1.46−5	1.49−5	1.55−5							
27	9.63−6	9.80−6		1.01−5								
28	6.60−6	6.70−6		6.92−6								

spin–spin interaction only leads to small differences (less than 11%) for the whole series, and for $Z > 10$ they are less than 5%. Similarly, the CI from $n = 4$ configurations only makes differences greater than 5% for the specific case of $Z = 6$. Regarding the branching ratio, it is seen that although the $n = 4$ configurations make little difference (except again for the neutral) the inclusion of the spin–spin contribution causes a large decrease at low Z from those obtained by including only the one-body relativistic corrections (approximation A′), which as expected tend to the value of 3 at low Z discussed by Ellis & Martinson (1984). These findings fully support the earlier conclusion by Fleming & Brage (1997) regarding the sensitivity of B to the Breit interaction in O III. As discussed above, the relative magnitude of the spin–spin contribution decreases along the sequence, and by $Z = 20$ its effects have been reduced to less than 5%.

The best present A-values are compared with other calculations in Tables 8–10 and in Fig. 3. In the case of $A(^5S^o_2 - ^3P_J)$, differences greater than 5% between the MCHF dataset and the present are found for $Z < 12$, growing to $\sim 20\%$ for $Z < 8$. However, the excellent agreement (better than 3%) between present data and those by Brage et al. (1997) and Fleming & Brage (1997) for $Z = 7, 8$ in the SCIV3 method gives us confidence in the accuracy of the present A-values for these transitions even at low Z. Still, significant discrepancies are found with the other datasets (MCDF, SSTR and CIV3) throughout the sequence. Regarding the relatively smaller A-values for the $^5S^o_2 - {}^1D_2$ transition, differences greater than 20% are found with MCHF throughout the sequence reaching a factor of 3 for $Z = 6$. Such large discrepancies are difficult to explain. In relation to other theoretical datasets, differences larger than 20% are found with MCDF, SSTR and CIV3 for $Z < 20$. This comparison seems to indicate that the present A-values for this transition are probably not accurate to better than 20%.

Radiative lifetimes and branching ratios computed with the best present transition probabilities are compared with other theoretical results in Tables 11–12 and in Fig. 4. Recent measurements are also included in the tabulations. The best agreement (1%) is found with the SCIV3 results for N II and O III. Discrepancies larger than 5% are found with MCHF for $Z < 12$, but they increase up to 30% for $Z < 8$. By examining the branching ratios (Fig. 4b), it is apparent that MCDF and SSTR did not include the Breit interaction in their computations, and the former displays a questionable departure for $Z = 8$. Perhaps for this same reason their lifetimes are significantly higher than MCHF and present results for $Z < 12$. The CIV3 dataset contains data for $Z = 8$ that lead to a comparable branching ratio but a noticeably higher lifetime. From this outcome and a further comparison with the experimental results (see Tables 11–12), and in spite of the scatter found in the measured values, we are confident in assigning a 5% rating to the present results for $Z > 8$ and 10% otherwise.

Table 12. Comparison of the best present results for the branching ratio $B = A(^5S^o_2 - {}^3P_2)/A(^5S^o_2 - {}^3P_1)$ with other theoretical and experimental results. Keys for theoretical results as in Table 11. Keys for experimental results: BWG, Bridges et al. (1996); MBDW, Musielok et al. (1996); CGL, Curry et al. (1997). The experimental uncertainty is given by the digits in parentheses

	Theory								Experiment		
Z	Pres.	MCHF	SSTR	MCDF	CIV3	SCIV3	NS	HB	BWG	MBDW	CGL
6	2.29	2.42									
7	2.36	2.47				2.44		2.23	2.45(4)	2.24(6)	2.27(23)
8	2.44	2.52	2.94	3.50	2.49	2.49	2.46				
9	2.50	2.54		3.03							
10	2.50	2.54	2.85	2.87	2.52						
11	2.48	2.52		2.77							
12	2.44	2.47	2.71	2.69	2.45						
13	2.38	2.41		2.60							
14	2.31	2.33	2.52	2.50	2.32						
15	2.21	2.24		2.38							
16	2.11	2.14	2.29	2.26							
17	1.99	2.02		2.12							
18	1.86	1.89	2.01	1.98							
19	1.73	1.76		1.84							
20	1.59	1.63	1.72	1.69	1.63						
21	1.46	1.49		1.55							
22	1.33	1.36	1.44	1.41							
23	1.20	1.24		1.27							
24	1.08	1.12		1.15							
25	0.97	1.02	1.06	1.04							
26	0.88	0.92	0.97	0.93	0.92						
27	0.79	0.83		0.85							
28	0.72	0.76		0.77							

4. Conclusions

We have performed a detailed study of the radiative decay properties of the $^5S^o_2$ metastable state in the carbon sequence. Ample evidence has been provided to support the conclusion by Fleming & Brage (1997) regarding the importance of the Breit interaction in obtaining accurate results for the low Z members and to illustrate its isoelectronic trend as theoretically predicted by Jones (1970). An extensive comparison with previous datasets for this sequence has allowed us to assign accuracy ratings to the present A-values. The transitions to the ground term are given a 10% ranking for $Z \leq 8$ and 5% for $Z > 8$ whereas the transitions to the $^1D_2$ are not accurate to more than 20%. We therefore assert that the present dataset, that will be included in the public databases of the IP, is the most reliable to date. Also, we would welcome further theoretical and experimental benchmarks that would clarify the inconclusive situation regarding the lifetimes and branching ratios for $Z < 8$.

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