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Accurate f values for N I and astrophysical implications

ABSTRACT

Two independent and accurate theoretical methods have been used (CIV3 and MCHF) for firmly establishing the oscillator strength scale of the infrared $\Delta n = 0$ transitions of N I. A refined value of the solar abundance of nitrogen is deduced from the CIV3 results: A(N) = 7.99 $\pm$ 0.04, in the usual logarithmic scale where the H abundance is 12.00.

INTRODUCTION

An accurate knowledge of CNO abundances in the sun is important for several reasons. Beside of the fact that they constitute a critical test of stellar evolution, the solar abundances remain the primary source of information for cosmic abundances and are often considered as standards for stellar composition. Moreover, due to the fact that these elements are basically volatile and incompletely condensed in meteorites, the sun remains the only source of information for the solar system abundances. The abundance value of nitrogen deduced in previous investigations (Lambert, 1968, 1978) suffered from the lack of an accurate scale of oscillator strengths. The main aim of this study is to provide such an accurate scale of f values for the $\Delta n = 0$ transitions of solar interest and hence to assess definitely the solar abundance value derived from allowed N I transitions.

CIV3 CALCULATIONS

The 12 lines used for the solar analysis (see Table 1) involve the 3 configurations $2s^2 2p^2 n\ell$ ($n\ell$ = 3s,3p,3d). The CI calculations have been performed using an orthogonal basis set (1s,2s,3s,4s,5s, 2p,3p,4p,3d,4d,5d,4f,5f,5g) which, except for the Slater type orbitals 4p,5f, had already been obtained previously (Hibbert *et al.*, 1985). Configuration interaction has been considered for the configurations $2s^2 2p^2 ns$, $2s^2 2p^2 nd$, $2s^2 2p3pns, 2p^4 nd$ (n=3–5), $2s^2 2p^2 5g$, $2p^4 ns$ (n=2–5), $2s2p^3 np$ (n=3,4) and $2s2p^3 4f$ for the even parity. For the odd parity, the configurations $2s^2 2p^3$, $2s^2 2p^2 np$, $2p^4 np$ (n=3,4), $2s^2 2p^2 nf$ (n=4,5), $2s2p^3 ns$, $2s2p^3 nd$ (n=3-5) and $2p^5$ have been retained. This gives rise to 157 and 151 CSF's respectively including all the coupling schemes. Another approach allowed in CIV3 and adopted here consists in making adjustments to the diagonal matrix elements to achieve an accurate energy spitting between the energy states. The inclusion of relativistic effects is done in the Breit-Pauli approximation including the spin-orbit, spin-other-orbit, spin-spin, mass correction and Darwin terms, and keeping the same adjustments as those found in the LS coupling.

MCHF RESULTS

The wave functions obtained with the CIV3 code include near-degeneracy and semi–internal correlation but do not retain external correlation effects. With the MCHF package, we used the notion of "reference set" for generating the wave function expansion, considering all possible single and double excitations which can be generated from the (2p,3s,3p,3d,4s,4p,4d,4f, 5s,5p,5d) virtual orbital basis set. The expansion sizes are quite large reaching 1333 CSF's for the $3p\ ^2D^o$ wave functions. Another major difference with CIV3 lies in the form of the radial distributions defining the one–electron orbitals, which are numerical (instead of analytical) and found by solving the MCHF equations. The Breit–Pauli calculations (MCHF+BP) of the transition probabilities will be performed in the near future and more details about the CIV3 and MCHF calculations themselves will be published at that time.

SOLAR ANALYSIS

The sample of the 12 infrared lines which was retained for the solar analysis is presented in Table 1 together with the relevant atomic (CIV3 gf values in the length and velocity formalisms) and solar data. For the 7 lines blended with CN, the CN weak contributions as calculated by Lambert (1978) were deduced from the center-of-disk equivalent widths. A classical LTE method of direct integration of the profiles was used for the analysis (see e.g. Biémont *et al.*, 1981) with the Holweger and Müller (1974) solar model. The mean abundance result, A(N) = 7.99 $\pm$ 0.04, corresponding to the mean of the length and velocity CIV3 f values, does agree very well with the abundance value reported by Lambert (1978) but with the basic difference that the scale of oscillator strength is now firmly established. This mean abundance result is slightly, though significantly lower than the result proposed by Anders and Grevesse (1989) (A(N) = 8.05 $\pm$ 0.04) and deduced from molecular lines.

REFERENCES

Anders,E., Grevesse,N., 1989 – Geochim. Cosmochim. Acta **53**, 197

Biémont,E., Grevesse,N., Hannaford,P., Lowe,R.M., 1981 – Astrophys.J. **248**, 67

Delbouille,L., Neven,L., Roland,G., 1973 - Photometric Atlas of the Solar Spectrum λ 3000 to λ 10000 - Institut d' Astrophysique - Université de Liège

Hibbert,A., Dufton,P.L., Keenan,F.P., 1985 – Mon. Not. R. Astr. Soc. **213**, 721

Table 1 : N I transitions used for the solar analysis.

λ_{lab} (a)	λ_{sun} (b)	transition	E_{low} (c)	Weight	W_λ (d)	$\log gf^{(e)}$ L	V	A_N (f)
7442.293	.23+	$3s\,^4P_{3/2} - 3p\,^4S^o_{3/2}$	10.33	2	2.7*	−0.387	−0.463	7.97
7468.307	.27+	$3s\,^4P_{5/2} - 3p\,^4S^o_{3/2}$	10.33	2	4.9	−0.171	−0.248	8.04
8216.345	.31	$3s\,^4P_{5/2} - 3p\,^4P^o_{5/2}$	10.34	1	8.7	0.146	0.089	7.96
8683.401	.39	$3s\,^4P_{3/2} - 3p\,^4D^o_{5/2}$	10.33	2	8.1*	0.115	0.102	7.89
8718.726	.77	$3s\,^4P_{5/2} - 3p\,^4D^o_{5/2}$	10.34	1	4.3*	−0.338	−0.347	8.02
9392.789	.78	$3s\,^2P_{3/2} - 3p\,^2D^o_{5/2}$	10.69	2	9.5*	0.328	0.378	7.97
8629.238	.17	$3s\,^2P_{3/2} - 3p\,^2P^o_{3/2}$	10.69	1	4.6*	0.090	0.078	7.91
8655.887	.86	$3s\,^2P_{3/2} - 3p\,^2P^o_{1/2}$	10.69	1	1.5	−0.603	−0.616	8.06
8594.005	3.99	$3s\,^2P_{1/2} - 3p\,^2P^o_{1/2}$	10.69	1	2.6*	−0.320	−0.332	8.04
10112.483	.53	$3p\,^4D^o_{5/2} - 3d\,^4D_{7/2}$	11.76	1	3.6	0.622	0.600	8.00
10114.644	.66	$3p\,^4D^o_{7/2} - 3d\,^4D_{9/2}$	11.76	2	5.4	0.778	0.755	8.05
10108.893	-	$3p\,^4D^o_{3/2} - 3d\,^4D_{5/2}$	11.75	2	2.5	0.443	0.420	7.99

(a) Laboratory wavelength (in Å) from Moore (1975)
(b) Solar wavelength (in Å) from Moore *et al.* (1966) (+) or from Swensson *et al.* (1970)
(c) Lower excitation potential (in eV)
(d) Equivalent width (in mÅ as measured on the Jungfraujoch spectra (Delbouille *et al.*, 1973); ⋆ CN contribution deduced (see text)
(e) $\log gf$ as obtained in this work in the length (L) or velocity (V) formalisms
(f) Abundance in the logarithmic scale ($A_N = \log \frac{N_N}{N_H} + 12.00$) calculated with the HM model and the mean of gf_L and gf_V.

Holweger,H., Müller,E.A., 1974 - Solar Phys. **39**, 19

Lambert,D.L., 1968 - Mon. Not. R. Astr. Soc. **138**, 143

Lambert,D.L., 1978 - Mon. Not. R. Astr. Soc. **182**, 249

Moore,C.E., 1975 - Selected Tables of Atomic Spectra - NSRDS - NBS 3, Section 5

Moore,C.E., Minnaert,M.G.J., Houtgast,J., 1966, The Solar Spectrum 2935 Å to 8770 Å - NBS Monograph 61

Swensson,J.W., Benedict,W.S., Delbouille,L., Roland,G., 1970, - The Solar Spectrum from λ 7498 to λ 12016 - Mem. Soc. Roy. Sci. Liège - Spec. Vol. 5

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