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Astron. Astrophys. 54, 757—764 (1977)

ASTRONOMY AND ASTROPHYSICS

Remarks on Atomic Partition Functions, the Example of Tin*

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Received July 17, 1974, revised July 20, 1976

Summary. In this paper problems concerning the calculations of the atomic-partition-function U for elements of complex internal structure (e.g. elements of iron group) are discussed. The program is formulated in detail as to take into account every energy level realizable in given physical conditions, including the levels lying above the *normal* ionization energy. It was found, with example of tin, that the contribution of these highly excited levels to the U-levels is substantial in a wide range of physical conditions. Our numerical values of the partition functions for Sn I, Sn II and Sn III differ considerably from those obtained by use of approximations given by other authors. The U-values recommended in this paper are given in the temperature range from 2000 to 40000 K for a lowering of ionization energy ranging from 0.05 to 2.00 eV.

Key words: partition functions — parent levels

1. Introduction

To determine the physical conditions in a plasma by spectroscopic methods, knowledge of the following quantities is necessary: (1) atomic constants, e.g. the transition probabilities and the Stark-effect spectral line constants and (2) quantities which can be functions of the state of the plasma, as e.g. the atomic partition functions U.

The dependence of numerical values of U on temperature T can easily be taken into account provided that data on the internal structure of an atom (energies E and statistical weights g of the levels) are known. The electron density N_e is a parameter which does not appear explicitly in the definition of the partition function, however, it is a main factor regulating (through the depression of the ionization energy ΔE) the number of energy levels on which the summing of the "statistical populations" is done. In fact, the physical conditions in the plasma may also affect the E and g values as well as the populations of the atomic states. [This concerns mainly the highly excited energy levels; cf. also Gündel (1970, 1971), Fischel and Sparks (1971).] Unfortunately, the presently published data, even for the unperturbed values of E and g, are not sufficiently complete for calculations (cf. tables of Moore, 1949–1958).

None of the current theories describes comprehensively the effect of the plasma on the atomic partition functions. Therefore, in order not to introduce the theoretical uncertainties into the final U-values, in this paper, a detailed program has been formulated on the basis of the conventional assumption that the whole effect of the plasma medium on the atomic partition function in r-th ionization state, $U^{(r)}$, may be adequately described by the parameter $\Delta E^{(r)}$ alone. The numerical values of $U^{(r)}$ were calculated for tin as an example for the discrete values of $\Delta E^{(r)}$, covering a wide range of the physical conditions in astrophysical and laboratory plasmas.

As it is well known, the tables of Moore contain the "observed" energy levels only. In this work, these tables have been supplemented for Sn I, Sn II and Sn III by several hundreds of levels in each ionization state, right up to the excitation energy which differs by less than 0.05 eV from the ionization energy of a level sequence based on a given parent level. The U-values obtained in this paper differ considerably from those which one obtains on the basis of Moore's levels only. [Such inaccurate calculations were performed until quite lately, e.g. in Boumans (1968), Galan et al. (1968).] Our results differ also from those calculated by neglecting the differences in the ionization energies of the sequences based on subsequent parent terms, as was done e.g. by Drawin and Felenbok (1965).

2. General Remarks

The atomic partition function is defined as follows (e.g. Griem, 1964; Traving et al., 1966; Drawin and Felenbok, 1965):

$$U^{(r)}(T, N_e) = \sum_{i=1}^{i_{\max}} g_i^{(r)} \exp(-E_i^{(r)}/kT), \quad (1)$$

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* This work was performed under the partial sponsorship of the U.S. National Bureau of Standards

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where $g_i^{(r)}$ are the statistical weights, $E_i^{(r)}$ the excitation energies of all bound states of the considered atom in the r-th ionization state ($r=0$ for neutral atoms, $r=1$ for singly charged ions, etc.). Upper limit, $i_{\max}$, is the number of levels whose excitation energies are smaller than the "ideal" ionization energy minus $\Delta E^{(r)}$ [this corresponds to the right-hand of the inequality (3) when $p=1$]. However, the above mentioned determination of $i_{\max}$ causes that the definition (1)—general until now—may be applied only to hydrogen-like systems where only a single parent level occurs. When energy levels belong to many different sequences (based on various parent levels), this cut-off procedure causes that all bound levels, the excitation energy of which is higher than the *normal* ionization energy (that is in the sequence based on the ground parent level), are not taken into account.

To avoid misunderstandings we define the atomic partition function for r-th ionization state explicitely:

$$U^{(r)}(T, N_e) = \sum_{p=1}^{p_{\max}} \sum_{i=1}^{i(p)_{\max}} g_{pi}^{(r)} \exp(-E_{pi}^{(r)}/kT) = \sum_{p=1}^{p_{\max}} U_p^{(r)}(T, N_e). \tag{2}$$

Here the set (pi) of the order numbers p and i (numbering the levels from the ground towards the higher ones) describe an eigenstate of the atom in the r-th ionization state: i represents three quantum numbers (nlj) of the optical electron and p the quantum state of the atomic core. $i(p)_{\max}$ is the number of all bound energy levels, $g_{pi}^{(r)}$ and $E_{pi}^{(r)}$ being the statistical weight and the excitation energy of the i-th state, in the sequence based on p-th parent level. The numbers $i(p)_{\max}$ result from the inequality

$$E_{pi}^{(r)} \leqq E_{p\infty}^{(r)} - \Delta E^{(r)}, \tag{3}$$

where $E_{p\infty}^{(r)}$ (the ionization energy in the p-th level sequence) is equal to the sum

$$E_{p\infty}^{(r)} = E_{1\infty}^{(r)} + E_p^{(r+1)}. \tag{4}$$

The value $p_{\max}$ in Equation (2) is the number of different parent levels that are realizable in given physical conditions. The number $p_{\max}$ results from the inequality of type (3) for $(r+1)$-th ionization state. Since for a fixed p-value the value of k is ascribed univocally, the upper limit of $E_{p\infty}^{(r)}$ for the k-fold excitation ($k=1, 2, \ldots, Z-r$, Z—the atomic number) can be written as follows:

$$E_{p\infty}^{(r)} \leqq \sum_{s=1}^{k} E_{1\infty}^{(r+s-1)}. \tag{5}$$

3. Calculation Technique

To calculate the energy of the quantum states of alkaline metals and alkaline-like ions, the simple model of the atomic core with the single valent electron is employed (cf. e.g. Condon and Shortley, 1963, Chapter 5). This model can also be used for more complex systems with one highly-excited electron. In this case, however, the quantum defect δ depends not only on the quantum numbers l and j of the valent electron but also on the quantum numbers describing the state of the atomic core.

At fixed values of the above-mentioned quantum numbers, the proper expression for this model:

$$E_{pn}^{(r)} = E_{p\infty}^{(r)} - (r+1)^2 Rhc/(n-\delta)^2, \tag{6}$$

adequately "reconstructs" the series of the same type (as e.g. $5s^2 5pnd\, {}^3D_2$). The quantities n, R, h and c in Equation (6) have their conventional meanings. Equation (6), after substitution of the quantities $a = ((r+1)^2 Rhc)^{-1/2}$ and $b = -\delta((r+1)^2 Rhc)^{-1/2}$, assumes the form:

$$E_{pn}^{(r)} = E_{p\infty}^{(r)} - (an+b)^{-2}. \tag{7}$$

For large values of n [for our purpose the Equation (7) is of interest for large n values only] this equation is equivalent to the Ritz formula [cf. e.g. paper of Meggers (1940), on tin].

The formulae (6) and (7) have been checked by the authors for many series of levels for different elements. (To this purpose the series for which in the Moore's tables n occurs in a wide range were chosen.) In Table 1 examples of this checking (left-hand of the table) and of working application (right-hand of the table) of both these formulae for tin are given. For illustration we have chosen the series ( )$ns\, {}^3P_1$ in which the levels are known up to $n=19$, but in the table the checking of both methods has been done with most unfavorable assumption that only the two lowest levels ($n=6$ and 7) are given. (In the working applications all accessible levels have been taken into account.) So, the values of E_2 and E_3 appearing in the Columns 4 and 6 result, respectively, from Equation (6) with the mean quantum defect of the two lowest levels, and from Equation (7) with parameters a and b defined by the same levels. $\Delta E_{1,2}$ and $\Delta E_{1,3}$ are the deviations from the corresponding Moore's values of E_1. In all examined cases such deviations were quite small (of the order of 1% or smaller). Consequently, we have assumed that both formulae may reliably be used to determine the "nonobserved" atomic levels.

In the right-hand of Table 1 a nontypical example is shown in which δ (Column 9) appreciably depends on the principal quantum number n. For comparison, the values with the asterisks in the Columns 9 and 11 have been obtained from the alternative linear relations: $\delta = cn + d$ (the quantum-defect method) and $(\Delta E_{p\infty,pn}^{(r)})^{-1/2} = an + b$ [the Ritz formula or Equation (7)] fitted to the Moore levels by the least-square method (see the lowest row in the table). The corresponding energies of "nonobserved" levels, determined by using both of the above-mentioned methods, are given in the

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Table 1. Examples of checking the accuracy of the applied methods (the left part of the table) and its working application to the Sn I levels (right part of the table)

$5s^2 5p(^2P_{1/2})ns\ ^3P_1$							$5s^2 5p(^2P_{3/2})nd\ ^1D_2$				
1	2	3	4	5	6	7	8	9	10	11	12
n	E_1	δ	E_2	$\Delta E_{1,2}$	E_3	$\Delta E_{1,3}$	E_1	$\delta = cn + d$	E_2	$(an+b)\times 10^3$	E_3
5							47145.7	2.4093		7.824	
6	34914.2	3.8765					55296.1	2.3403		11.052	
7	48222.1	3.8440						2.380*	58345.7	13.92*	58322.3
8	53020.6	3.7982	52833.1	187.5	52980.9	39.7		2.403*	59982.7	16.87*	59969.5
9	55156.0	3.8131	55080.8	75.2	55208.7	−52.7		2.427*	60945.1	19.82*	60932.4
10	56389.2	3.7890	56322.8	66.4	56427.5	−38.2	61534.2	2.4992		22.651	
11	57094.5	3.8371	57080.6	13.9	57165.9	−71.4	61963.0	2.5070		25.648	
12	57563.0	3.8938	57576.7	−13.7	57646.9	−83.9	62263.9	2.5167		28.638	
13	57899.0	3.9294	57919.1	−20.1	57977.6	−78.6	62483.1	2.5289		31.621	
14	58143.6	3.9616	58165.2	−21.6	58214.6	−71.0	62647.8	2.5431		34.598	
15	58324.3	4.0075	58348.1	−23.8	58390.3	−66.0	62774.6	2.5601		37.566	
16	58523.3	3.5592	58487.7	35.6	58524.1	−1.1	62871.2	2.6144		40.423	
17	58607.5	3.7468	58596.7	10.8	58628.3	−20.8	62954.2	2.6025		43.478	
18	58690.0	3.7735	58683.3	6.7	58711.2	−21.2	63018.1	2.6453		46.369	
19	58758.4	3.7804	58753.4	5.0	58778.0	−19.6	63072.6	2.6580		49.350	
20			58810.8		58832.9			2.685*	63117.4		63117.2
Mean		3.8293		26.8		−40.4		$c = 0.0202 \pm 0.0016$ $d = 2.273 \pm 0.023$		$a = 2.959 \pm 0.005$ $b = -6.863 \pm 0.068$	

Columns 10 and 12. [Note: in all cases in which Moore's tables were unsufficient for such calculations, each of the parameters c, d (or a, b) have been proportionally (with respect to the parameters in a known series) transferred from corresponding series in elements isoelectronic in relation to tin.]

The procedures of "individual" supplementation of the Moore tables are applicable (due to accessible data) only to level sequences based on the lowest parent levels ($p = 1, 2, \ldots, p_1$) which form the ground parent term or, at most, the ground parent configuration. The contributions of the remaining sequences ($p > p_1$) to the atomic partition function may be taken into account, as a whole, by assuming the similarity of their structure (in relation to the earlier mentioned sequences) and using the proper Boltzmann factors.

Thus, for $p > p_1$ the values of $U_p^{(r)}$ can be calculated according to the relation

$$U_p^{(r)} = \sum_{i=1}^{i_1(p)} g_{pi}^{(r)} \exp(-E_{pi}^{(r)}/kT) + \Delta U_p^{(r)}, \tag{8}$$

where

$$\Delta U_p^{(r)} = [g_p^{(r+1)}/g_q^{(r+1)}] \Delta U_q^{(r)} \exp[(E_q^{(r+1)} - E_p^{(r+1)})/kT]. \tag{8'}$$

Here q ($q \leqq p_1$) represents a comparative sequence for which

$$\Delta U_q^{(r)} = \sum_{i=i_1(q)+1}^{i(q)_{\max}} g_{qi}^{(r)} \exp(-E_{qi}^{(r)}/kT);$$

the quantities $i_1(p)$ and $i_1(q)$ are the numbers of atomic levels (in p and q sequences) from the ground state up to the (excluded) states of the same quantum numbers $n'l'$ of the optical electron.

The relation between $\Delta U_p^{(r)}$ and $\Delta U_q^{(r)}$ (8′) is strict if, at fixed numbers nl of the optical electron, a change $q \to p$ of the state of the atomic core does not change the electron-core interaction energy. In that case, the energy levels of the p sequence are shifted as a whole in relation to q sequence by the value $|E_p^{(r+1)} - E_q^{(r+1)}|$, and the statistical weights satisfy the relation $g_{pi}^{(r)}/g_{qi}^{(r)} = g_p^{(r+1)}/g_q^{(r+1)}$.

This condition is never realized. However, an error introduced into $U_p^{(r)}$ by the formula (8′) is minim when in both (p and q) sequences under consideration the maximal bounded energies are close one to another. It should be noted that $U^{(r)}$ values are of physical interest only in such a T-range that $E_{1\infty}^{(r)}/kT \gg 1$. Because for $p > p_1$ is $E_{pi}^{(r)} \gtrsim E_{1\infty}^{(r)}$ (except for a few of the lowest levels), the error contributed by $U_p^{(r)}$ to $U^{(r)}$ is always small.

The sequences further than some p (say, $p = p_2$), do not occur at all in Moore's tables. Consequently, for $p \geqq p_2$, the $U_p^{(r)}$ values are defined only by the second term on the right-hand of Equation (8). Since these sequences are based on highly excited energy levels [$E_{p2}^{(r+1)}$ is of the order of $E_{1\infty}^{(r)}$], they all may be referred—with adequate accuracy for the calculations—to one common comparative q sequence (e.g. the ground one

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Table 2. The atomic partition functions for Sn I

T [K]	Lowering of the ionization energy [eV]						
	0.05	0.10	0.25	0.50	0.75	1.00	2.00
2000	2.323	2.323	2.323	2.323	2.323	2.323	2.323
3000	3.380	3.380	3.380	3.380	3.380	3.380	3.380
4000	4.318	4.318	4.318	4.318	4.318	4.318	4.318
5000	5.136	5.136	5.136	5.135	5.135	5.135	5.135
5500	5.507	5.506	5.505	5.505	5.505	5.505	5.504
6000	5.860	5.855	5.853	5.852	5.852	5.851	5.850
6500	6.205	6.189	6.182	6.180	6.179	6.178	6.175
7000	6.557	6.515	6.498	6.492	6.490	6.488	6.482
7500	6.943	6.846	6.806	6.794	6.788	6.784	6.772
8000	7.396	7.196	7.113	7.090	7.079	7.071	7.050
8250	7.663	7.385	7.269	7.237	7.222	7.211	7.184
8500	7.966	7.586	7.429	7.385	7.365	7.351	7.317
8750	8.314	7.804	7.593	7.535	7.508	7.490	7.447
9000	8.714	8.040	7.762	7.687	7.652	7.629	7.575
9250	9.177	8.300	7.939	7.842	7.798	7.768	7.702
9500	9.713	8.587	8.125	8.001	7.945	7.908	7.828
9750	10.33	8.905	8.321	8.165	8.096	8.049	7.954
10000	11.05	9.258	8.528	8.335	8.249	8.193	8.078
10250	11.87	9.653	8.750	8.511	8.406	8.338	8.203
10500	12.82	10.09	8.986	8.695	8.568	8.486	8.328
10750	13.90	10.58	9.239	8.888	8.735	8.637	8.453
11000	15.13	11.13	9.510	9.090	8.908	8.793	8.578
11250	16.52	11.73	9.802	9.302	9.087	8.952	8.705
11500	18.10	12.41	10.12	9.525	9.274	9.116	8.833
11750	19.88	13.15	10.45	9.761	9.468	9.284	8.963
12000	21.87	13.98	10.82	10.01	9.670	9.459	9.094
12500	26.58	15.89	11.63	10.55	10.10	9.826	9.364
13000	32.40	18.20	12.57	11.16	10.57	10.22	9.644
13500	39.55	20.96	13.66	11.84	11.09	10.65	9.936
14000	48.29	24.26	14.91	12.60	11.66	11.11	10.24
14500	58.95	28.16	16.34	13.45	12.29	11.60	10.57
15000	71.94	32.78	17.98	14.40	12.97	12.14	10.91
15500	87.85	38.23	19.85	15.46	13.73	12.73	11.27
16000	107.4	44.67	21.98	16.64	14.56	13.37	11.65
16500	131.6	52.27	24.39	17.96	15.47	14.06	12.06
17000	161.6	61.28	27.14	19.43	16.46	14.81	12.49
17500	199.2	71.97	30.25	21.05	17.55	15.62	12.95
18000	246.4	84.70	33.78	22.86	18.75	16.50	13.44
18500	305.7	99.91	37.79	24.86	20.06	17.46	13.96
19000	380.5	118.1	42.34	27.09	21.49	18.50	14.51
19500	474.8	139.9	47.50	29.55	23.06	19.62	15.10
20000	593.6	166.2	53.37	32.28	24.76	20.84	15.72

where $q=1$). Then

$$\sum_{p=p_2}^{p_{\max}} U_p^{(r)} = \sum_{p=p_2}^{p_{\max}} [g_p^{(r+1)}/g_q^{(r+1)}] U_q^{(r)} \exp[(E_q^{(r+1)} - E_p^{(r+1)})/kT] = [U_q^{(r)}/g_q^{(r+1)}] \exp(E_q^{(r+1)}/kT) \cdot \left[U^{(r+1)} - \sum_{p=1}^{p_2-1} g_p^{(r+1)} \exp(-E_p^{(r+1)}/kT)\right]. \quad (9)$$

It is proper to add that for $q=1$ and $p_2=2$, the relation (9) reduces to the simple

$$U^{(r+1)}/U^{(r)} = g_1^{(r+1)}/U_1^{(r)}. \quad (10)$$

This relation is adequately accurate for $U^{(r)}$ calculations when $E_2^{(r+1)}/kT \gg 1$.

Recapitulation. In each ionization state under consideration the sequences of energy levels have been divided into three groups, the contributions to the atomic partition functions of which are defined in following terms: $\alpha^{(r)}$—for the sequences $p \leqq p_1$—by a discrete summation [cf. Eq. (2)], $\beta^{(r)}$—for $p_1 < p < p_2$—according to Equation (8), and $\gamma^{(r)}$—for the remaining sequences—by Equation (9). In all cases the Moore tables have served as preliminary data.

4. Results of the Numerical Calculations

In the present paper, numerical values of the atomic partition functions have been calculated for tin according to the described program, as an example.

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Table 3. The atomic partition functions for Sn II

T [K]	Lowering of the ionization energy [eV]						
	0.05	0.10	0.25	0.50	0.75	1.00	2.00
7500	3.771	3.771	3.771	3.771	3.771	3.771	3.771
8000	3.865	3.865	3.865	3.865	3.865	3.865	3.865
8250	3.910	3.910	3.910	3.910	3.910	3.910	3.910
8500	3.954	3.954	3.954	3.954	3.954	3.954	3.954
8750	3.996	3.996	3.996	3.996	3.996	3.996	3.996
9000	4.037	4.037	4.037	4.037	4.037	4.037	4.037
9250	4.078	4.078	4.078	4.078	4.077	4.077	4.077
9500	4.117	4.117	4.117	4.117	4.117	4.117	4.117
9750	4.156	4.156	4.156	4.156	4.156	4.156	4.156
10000	4.195	4.194	4.194	4.194	4.194	4.194	4.194
10250	4.233	4.232	4.232	4.232	4.232	4.232	4.232
10500	4.272	4.270	4.270	4.269	4.269	4.269	4.269
10750	4.310	4.308	4.307	4.307	4.307	4.307	4.306
11000	4.349	4.346	4.344	4.344	4.344	4.344	4.344
11250	4.388	4.384	4.382	4.382	4.381	4.381	4.381
11500	4.429	4.423	4.420	4.419	4.419	4.419	4.419
11750	4.470	4.462	4.458	4.457	4.457	4.457	4.456
12000	4.514	4.503	4.497	4.496	4.495	4.495	4.495
12500	4.606	4.587	4.577	4.575	4.574	4.574	4.573
13000	4.710	4.677	4.661	4.657	4.656	4.655	4.654
13500	4.830	4.776	4.750	4.744	4.742	4.741	4.739
14000	4.971	4.887	4.846	4.836	4.833	4.832	4.829
14500	5.140	5.012	4.949	4.935	4.930	4.928	4.924
15000	5.345	5.155	5.062	5.041	5.034	5.031	5.025
15500	5.596	5.321	5.185	5.155	5.145	5.141	5.132
16000	5.903	5.513	5.322	5.279	5.265	5.259	5.247
16500	6.280	5.738	5.472	5.414	5.394	5.386	5.370
17000	6.741	6.001	5.639	5.560	5.533	5.522	5.501
17500	7.304	6.310	5.825	5.719	5.683	5.668	5.641
18000	7.988	6.673	6.031	5.892	5.845	5.826	5.791
18500	8.814	7.098	6.261	6.081	6.020	5.995	5.950
19000	9.809	7.594	6.518	6.286	6.208	6.176	6.120
19500	11.00	8.174	6.803	6.509	6.411	6.371	6.301
20000	12.42	8.848	7.121	6.752	6.629	6.579	6.492
21000	16.08	10.54	7.871	7.304	7.117	7.041	6.911
22000	21.16	12.79	8.798	7.955	7.679	7.568	7.381
23000	28.16	15.76	9.843	8.724	8.328	8.169	7.904
24000	37.81	19.66	11.35	9.629	9.074	8.853	8.487
25000	51.23	24.77	13.09	10.70	9.931	9.630	9.133
26000	70.23	31.50	15.22	11.95	10.92	10.51	9.848
27000	97.71	40.40	17.85	13.42	12.05	11.51	10.64
28000	138.3	52.33	21.10	15.16	13.35	12.65	11.51
29000	199.6	68.51	25.14	17.22	14.85	13.94	12.48
30000	293.3	90.80	30.18	19.65	16.57	15.42	13.55

The results are entered in Tables 2–4 as functions of two parameters: (1) of the temperature T from 2 to 20, from 7.5 to 30, and from 8.5 to 40 thousands of kelvins for Sn I, Sn II and Sn III, respectively, and (2) of the lowering of the ionization energy $\Delta E^{(r)}$ which in all cases assumes seven values ranging from 0.05 to 2.00 eV. The range of physical conditions under consideration comprises the majority of astrophysically and physically interesting cases. [Note: for temperatures lower those mentioned above, the $U^{(r)}$ values can be obtained, exact to four digits, by taking into account the levels of the lowest ground term only.]

As it is seen in Equation (9), to calculate the $U^{(r)}$ value the value of $U^{(r+1)}$ in the same physical conditions is necessary. Therefore, our calculations start from $U^{(5)}$ in taking into account Moore's levels only. (For $U^{(5)}$, this is a proper approximation up to $4\,10^4$ K.) Then, $U^{(4)}$ values were calculated from Equation (10), it being adequate here. Subsequently, these last values served for the calculation of $U^{(3)}$. The values of $U_1^{(4)}$ appearing in this case in Equation (10), have been calculated by discrete summation over the basic sequence after its supplementation according to Equation (6).

To calculate the numerical values of $U^{(3)}$, the level-sequences have been divided into the following groups (with the same designations as in the Recapitulation of the former Section): $\alpha^{(3)}$—the sequence which derives from the ground parent term $4d^{10}5s\,^2S_{1/2}$; $\beta^{(3)}$—both

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Table 4. The atomic partition functions for Sn III

T [K]	Lowering of the ionization energy [eV]						
	0.05	0.10	0.25	0.50	0.75	1.00	2.00
8500	1.001	1.001	1.001	1.001	1.001	1.001	1.001
9000	1.001	1.001	1.001	1.001	1.001	1.001	1.001
9500	1.002	1.002	1.002	1.002	1.002	1.002	1.002
10000	1.003	1.003	1.003	1.003	1.003	1.003	1.003
10500	1.004	1.004	1.004	1.004	1.004	1.004	1.004
11000	1.005	1.005	1.005	1.005	1.005	1.005	1.005
11500	1.007	1.007	1.007	1.007	1.007	1.007	1.007
12000	1.010	1.010	1.010	1.010	1.010	1.010	1.010
12500	1.013	1.013	1.013	1.013	1.013	1.013	1.013
13000	1.017	1.017	1.017	1.017	1.017	1.017	1.017
13500	1.021	1.021	1.021	1.021	1.021	1.021	1.021
14000	1.027	1.027	1.027	1.027	1.027	1.027	1.027
14500	1.033	1.033	1.033	1.033	1.033	1.033	1.033
15000	1.039	1.039	1.039	1.039	1.039	1.039	1.039
15500	1.047	1.047	1.047	1.047	1.047	1.047	1.047
16000	1.056	1.056	1.056	1.056	1.056	1.056	1.056
16500	1.066	1.065	1.065	1.065	1.065	1.065	1.065
17000	1.076	1.076	1.076	1.076	1.076	1.076	1.076
17500	1.088	1.088	1.088	1.088	1.088	1.088	1.088
18000	1.101	1.100	1.100	1.100	1.100	1.100	1.100
18500	1.114	1.114	1.114	1.114	1.114	1.114	1.114
19000	1.130	1.129	1.128	1.128	1.128	1.128	1.128
19500	1.146	1.145	1.144	1.144	1.144	1.144	1.144
20000	1.164	1.162	1.161	1.161	1.161	1.161	1.160
21000	1.206	1.200	1.198	1.197	1.197	1.197	1.197
22000	1.256	1.245	1.240	1.239	1.238	1.238	1.238
23000	1.320	1.297	1.287	1.285	1.284	1.284	1.283
24000	1.404	1.359	1.341	1.336	1.335	1.335	1.333
25000	1.517	1.434	1.402	1.393	1.391	1.390	1.388
26000	1.673	1.528	1.472	1.457	1.453	1.452	1.448
27000	1.890	1.647	1.554	1.528	1.521	1.519	1.514
28000	2.195	1.800	1.649	1.608	1.597	1.594	1.585
29000	2.624	2.000	1.763	1.698	1.681	1.676	1.662
30000	3.227	2.262	1.899	1.801	1.775	1.768	1.747
31000	4.073	2.609	2.065	1.918	1.881	1.870	1.840
32000	5.263	3.068	2.268	2.054	2.000	1.984	1.941
33000	6.940	3.677	2.518	2.212	2.136	2.112	2.052
34000	9.320	4.486	2.827	2.398	2.290	2.258	2.175
35000	12.73	5.566	3.211	2.615	2.468	2.423	2.310
36000	17.65	7.014	3.690	2.872	2.672	2.611	2.459
37000	24.83	8.963	4.287	3.177	2.909	2.826	2.625
38000	35.37	11.60	5.036	3.540	3.185	3.073	2.810
39000	50.90	15.21	5.976	3.974	3.506	3.358	3.017
40000	73.82	20.14	7.162	4.492	3.882	3.687	3.248

sequences based on parent term $4d^{10}5p\,^2P^0_{1/2,\,3/2}$; $\gamma^{(3)}$—the remaining.

In $\beta^{(3)}$, both sequences were referred to the sequence mentioned in $\alpha^{(3)}$; the discrete summation was made up to $n'=6$, $l'=0$, i.e. over the levels of the configuration $5p^2$ in the sequences under consideration and, respectively, over the levels of $5s^2$ and $5s5p$ configurations in the comparative sequence $\alpha^{(3)}$.

The division to calculate $U^{(2)}$ was: $\alpha^{(2)}$—the sequence based on the ground parent term $4d^{10}5s^2\,^1S_0$; $\beta^{(2)}$—four sequences based on the levels of the configuration $5s5p$; [In these sequences the discrete summation was made over the levels of the configuration $5s5p^2$ and, respectively, over the levels of the configuration $5s^25p$ in the comparative sequence $\alpha^{(2)}$.] $\gamma^{(2)}$—the remaining sequences.

The division of the parent levels for the calculation of $U^{(1)}$ was: $\alpha^{(1)}$—both levels of the ground parent term $5s^25p\,^2P^0_{1/2,\,3/2}$; $\beta^{(1)}$—all the levels of the configuration $5s5p^2$ and the levels $5s^26s\,^2S_{1/2}$, $5s^25d\,^2D_{3/2,\,5/2}$, $5s^26p\,^2P^0_{1/2,\,3/2}$; $\gamma^{(1)}$—the remaining.

In $\beta^{(1)}$ the discrete summation was performed over all the levels of the $5s5p^3$ configuration (belonging to the sequences based on the parent levels of the $5s5p^2$ configuration) and, respectively, over the corresponding levels of the $5s^25p^2$ configuration in the comparative

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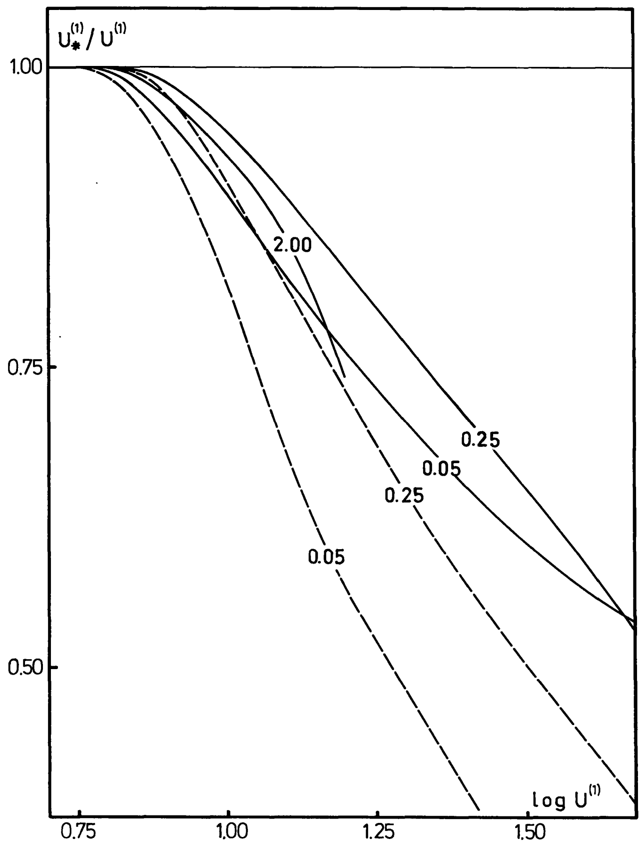

Fig. 1. The ratio $U_*^{(1)}/U^{(1)}$ vs. $\log U^{(1)}$ (both U-values being for the same physical conditions), where $U^{(1)}$ are the values of the partition functions recommended in this paper. The solid curves correspond to $U_*^{(1)}$ calculated by the technique of Drawin and Felenbok; the dashed curves to $U_*^{(1)}$ values calculated on the basis of the Moore levels only. The numbers on the curves are the values of the lowering of the ionization energy, $\Delta E^{(1)}$, in eV. For $\Delta E^{(1)}=2.00$ eV the curves obtained from both approaches are identical. The separations of the curves occurs for temperatures ranging from 6500 K upwards

sequences $\alpha^{(1)}$. The remaining sequences have been taken into account, according to Equation (8), by putting $U_p^{(r)}=\Delta U_p^{(r)}$. The sequences of the parent levels: $5s5p^2\,{}^4P_{1/2,\,3/2}$, $5s^26s\,{}^2S_{1/2}$, $5s5p^2\,{}^2D_{3/2}$, $5s^25d\,{}^2D_{3/2}$, $5s^26p\,{}^2P^0_{1/2}$, $5s5p^2\,{}^2S_{1/2}$, $5s5p^2\,{}^2P_{1/2}$ have been taken into account in relation to the sequence of the lowest ground parent level $5s^25p\,{}^2P^0_{1/2}$; the remaining sequences in $\beta^{(1)}$—in relation to the sequence based on the parent level $5s^25p\,{}^2P^0_{3/2}$. (As a criterion of the ascription, the j-quantum number was used.)

It is well known that in the case of configurations with equivalent electrons difficulties occur in the determination of the parentage of terms and—all the more—of energy levels (cf. e.g. Slater, 1960; Judd, 1963; Sobel'man, 1963, on the fractional parentage coefficients). Therefore, in the groups $\beta^{(r)}$ in which configurations with the equivalent electrons p^2 and p^3 occur, the contributions $\Delta U_p^{(r)}$(8′) have been defined for energy levels lying above those of the configurations under consideration. By summing over p sequences ($p>p_1$) in both sides of Equation (8), one can take into account the contributions to $U^{(r)}$ of all levels belonging to these sequences, without determination of the parentage of the levels of the configuration with the equivalent electrons.

Out of the groups $\alpha^{(r)}$, only $\alpha^{(1)}$ asks for a comment. The levels of the configuration with equivalent electrons $5s^25p^2$ belong to both sequences included in $\alpha^{(1)}$. In this case the parent term is known; however, difficulties occur in the determination of the level parentage within all three *daughter* terms. Since each of the sequences from $\alpha^{(1)}$ becomes a comparative one for the sequences in $\beta^{(1)}$, the values of $U_1^{(1)}$ and $U_2^{(1)}$ should be known separately. Therefore, the levels of the configuration $5s^25p^2$ have been included into both sequences in $\alpha^{(1)}$ with fractional weights. The numerical values of these weights are equal to the product of the statistical weight of the level and the proper (normalized to 1) "fractional parentage coefficient" for this level. We have assumed that the ratio of these coefficients is equal to that of the statistical weights of both parent levels. So, for the parent term under consideration we have obtained the following values of the coefficients: 1/3 and 2/3 for the parent levels ${}^2P^0_{1/2}$ and ${}^2P^0_{3/2}$, respectively.

In all ionization states, the sequences $\alpha^{(r)}$ were supplemented by the levels (missing in the Moore tables) right up to the energies $E_{p\infty}^{(r)}-\Delta E^{(r)}$. If in any given level-series at least three energy levels were accessible, then the relation (7) was used; in other cases—the relation (6). For some of the quantum states of Sn I, with $l=3$ and 4, the values of δ were transferred (cf. Note in the Section 3) from elements isoelectronic in relation to neutral tin. We have found that δ rapidly decreases to zero when l increases. Therefore, for $l>5$ we assumed generally $\delta=0$.

5. Conclusions

In this paper problems concerning the atomic-partition-function calculations for elements of complex internal structure (as e.g. the elements of iron group) are discussed.

A detailed program is formulated to take into account all energy levels realizable in given physical conditions. In particular, this concerns energy levels which lie—due to the variety of ionization energies in the level sequences deriving themselves from different parent levels—above the *normal* ionization energy. It has been found that the contribution of these highly excited levels to the U-values is substantial in a wide range of physical conditions, particularly in high T and low N_e (of the order of this in stellar atmospheres). In this range, not only the approximation of the parti-

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tion functions by the weight of the ground term only (Allen, 1973) or by summing on the populations of the Moore levels (as e.g. Boumans, 1968), but also the approach of Drawin-Felenbok (1965) in which the energy levels are supplemented below and generally ignored above the *normal* ionization energy, becomes inadequate (cf. Fig. 1).

In the same physical conditions the effect under consideration is greater as the ionization state of the element is lower. That is of great importance when one interprets the spectral line intensities by the Boltzmann and Saha-Eggert laws, e.g. in determining the stellar abundances or in measuring the transition probabilities from the emission lines of laboratory plasmas. It is proper to add that the problem of ionization-energy variety (in the same state of a complex element) and its importance for derived U-values and the ionization balance may be overlooked completely, when for stellar abundance computations or for A_{ki} measurements the procedures explicitly involving the differences between the ionization and the excitation energies are used without discrimination.

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