Tables of the partition functions for nickel, Ni I – Ni X.

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ABSTRACT

We present extensive tables of the atomic partition function (APF) for nickel ions, Ni I – Ni X. Partition functions are given over wide range of temperature, $10^3\,\mathrm{K} < T < 10^6$ K, and lowering of ionization energy ($0.001\,\mathrm{eV} < LIE < 5.0$ eV), both taken as independent variables. Our APF take into account all energy levels predicted by quantum mechanics, including autoionization levels. The tables can be applied for the computations of model stellar atmospheres and theoretical spectra over very wide range of spectral classes, from the coolest K–M dwarfs up to the hottest main sequence, giant, and white dwarf stars. This include also model spectra of supersoft X-ray sources and accretion discs in interacting binaries.

Our tables are available at `http://www.astrouw.edu.pl/∼acta/acta.html` (Acta Astronomica Archive), and `http://draco.uni.opole.pl/Halenka.html`.

Key words: Atomic data – Plasmas – Stars: atmospheres

1. Introduction

The knowledge of realiable atomic partition functions (APF) is of extreme importance for the determination of ionization balance in astrophysical plasmas. In particular, partition functions are coefficients of the Saha-Eggert equations describing ionization states of elements in stellar atmospheres (equation of state for plasma in Local Thermodynamic Equilibrium). Therefore the knowledge of numerical values of the APF is essential for computations of model stellar atmospheres and theoretical spectra, and for correct interpretation of intensities of absorption spectral lines and abundance determination of elements in stellar atmospheres.

Given value of the partition function U for a particular ion depends on gas temperature T, and the local electron concentration N_e. Temperature enters partition function by its definition (e.g. Griem 1964, Drawin and Felenbok 1965, Traving et al. 1966):

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

where the sum is taken over discrete energy levels of statistical weight i and excitation energies E_i. In vacuum ($N_e = 0$) the number of bound levels i_{max} is infinite, and therefore the above series always diverges.

In real plasma, however, interaction between the atom of interest and surrounding free electrons and ions (plasma effects) cause, that bound levels of very high excitation energies move to continuum and no longer contribute to the partitiion function. Therefore the series in Eq. (1) reduces to finite number of terms, and value of U is also finite and is strongly dependent on the electron concentration N_e. In general, the larger is N_e the lower is both number of bound energy levels i_{max} in Eq. (1), and the value of U.

There exist a large number of papers, which present tables of rather approximate (or even schematic) partition functions (APF) for elements, including nickel ions (Drawin and Felenbok 1965; Traving et al. 1966; Irwin 1981, for example). The latter paper present fitting formulae for APF of Ni I – Ni III, for temperatures $T \leq 16000$ K. The widely used computer code Tlusty 195 for computations of NLTE model stellar atmospheres (Hubeny and Lanz 1992, 1995) contains FORTRAN subroutine computing APF of Ni IV – Ni IX by direct summation over all *observed* energy levels of these ions. However, all these partition functions for Ni ions depend only on temperature T, and no level dissolution with increasing density is included here. The latter implies, that the set of energy levels was not complete there.

Quality of given tables of partition functions depend on (i) accuracy and completeness of energy levels included in Eq. (1), and (ii) realiability of the assumed theory of emitter-plasma interactions. Emitter-plasma interactions cause that the series in Eq. (1) is finite.

Unfortunately, none of the currently existing theories describe correctly effects of charged particles in plasma on the atomic partition functions, cf. also Hummer and Mihalas (1988).

Taking this into account we have decided to compute and present tables of the partition functions taking into account all energy levels predicted by quantum mechanics, including also levels lying above the so called *normal ionization energy* (autoionization levels). Moreover, our computations are more physically correct, since the APF depend on both temperature T and electron concentration N_e, through tabulated values of lowering of the ionization energy (LIE). The method of APF calculations is briefly described in the following Section. Detailed description of this method was presented in a series of papers by Halenka and Grabowski (1977, 1984, 1986), Halenka (1988, 1989), and Madej et al. (1999).

2. Computation of the atomic partition functions

We define the atomic partition function of r-th ionization state by the equation

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

cf. Halenka and Grabowski (1977). Here the set (pi) with the indices p and i (ordering of levels from the ground level upwards in energy scale) describes an eigenstate of the atom in the r-th ionization state. Index i represents three quantum numbers (nlj) of the optical electron, and p represents the quantum state of the atomic core. Index $i(p)_{max}$ is the number of all bound energy levels, $g_{pi}^{(r)}$ and $E_{pi}^{(r)}$ denote statistical weight and excitation energy of the i-th state, in the sequence based on the p-th parent level. Numbers $i(p)_{max}$ result from the inequality

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

where $\Delta E^{(r)}$ denotes the lowering of the ionization energy LIE, and $E_{p\infty}^{(r)}$ is the ionization energy in the p-th level sequence. The latter quantity is equal to the sum

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

The quantity $E_p^{(r+1)}$ denotes the energy of the atomic core after ionization, $r \to r+1$. Index p_{max} is the number of different parent levels which can be realized in given physical conditions. The number p_{max} results from the inequality similar to Eq. (3), written for the $(r+1)$-th ionization state. Since for a fixed value of p the number k is assigned unambigously, then the upper limit of $E_{p\infty}^{(r)}$ for the k-fold excitation ($k = 1, 2, \ldots, Z-r$, where Z is the atomic number) can be written as follows

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

Following Eq. (3) we have computed extensive tables of the APF for nickel in the 10 lowest ionization states, Ni I – Ni X. Excitation energies and statistical weights of the "observed" levels available for nickel ions were taken from Kurucz (1994). We have added to our partition functions contribution from many energy levels predicted by quantum mechanics, but missed in his catalogue. This include also many autoionizing levels. Exact description of the method of adding of missing levels is given in Halenka and Grabowski (1977, 1984).

In practical model atmosphere calculations one has to estimate the lowering of ionization energy for nickel as function of temperature T and electron concentration N_e. Such a relation has to result from the model describing plasma-emitter interaction. Unfortunately, none of the existing models is satisfactory enough (Hummer and Mihalas 1988). We suggest use of the approximate relation between the LIE and N_e

$$_{\triangle}\chi = Ze^2/D = 3 \times 10^{-8} Z N_e^{1/2} T^{-1/2} \quad [\mathrm{eV}] \tag{6}$$

(Eq. 9-106 of Mihalas, 1978), where $D = 4.8\,(T/N_e)^{1/2}$ [cm] is the Debye length in hydrogen dominated plasma. However, other relations of this type are also given by Drawin and Felenbok (1965).

3. Results

As the ilustration of our recommended results, Fig. 1 presents run of APF for Ni V and temperatures corresponding to atmospheres of hot white dwarf stars, for various values of LIE taken as free parameter (solid lines). Numerical values of APF for Ni V are listed in Table 1. For a comparison, we have computed also partition functions taking into account so called *observed* levels (single dashed line). One can easily note, that our recommended partition functions are significantly larger than the latter functions.

Partition functions for nickel are arranged in 10 ASCII tables, where each table corresponds to a single ion. Complete set of these data is available from Acta Astronomica Archive , `http://www.astrouw.edu.pl/~acta/acta.html`,
or `http://draco.uni.opole.pl/Halenka.html`.

Entries of a table are decimal logarithms of the APF. They are tabulated at 62 discrete temperatures, spaced at nonequidistant intervals, $10^3 \leq T \leq 10^6$ K, and at 9 arbitrarily assumed values of the lowering of ionization energy (LIE = 0.001, 0.003, 0.010, 0.030, 0.100, 0.300, 1.000, 3.000, and 5.000 eV). Both T and LIE points remain identical in all 10 tables of APF, to ensure homogeneity of the data.

We are aware, that some values of T and LIE in our tables do not correspond to conditions met in astrophysical plasma. However, the extend of all tables ensures, that they cover practically all T and LIE expected in stellar atmospheres of any type, excluding atmospheres of known neutron stars (temperatures $T \geq 10^6$ K).

Tables presented in this paper are based on the most complete set of energy levels actually available. Moreover, our partition functions are sensitive for plasma interactions, i.e. they strongly depend on the lowering of ionization energy, which is expected in plasma. Our APF tend to diverge for the lowering of ionization energy approaching zero, which is the fundamental property of the partition functions in general.

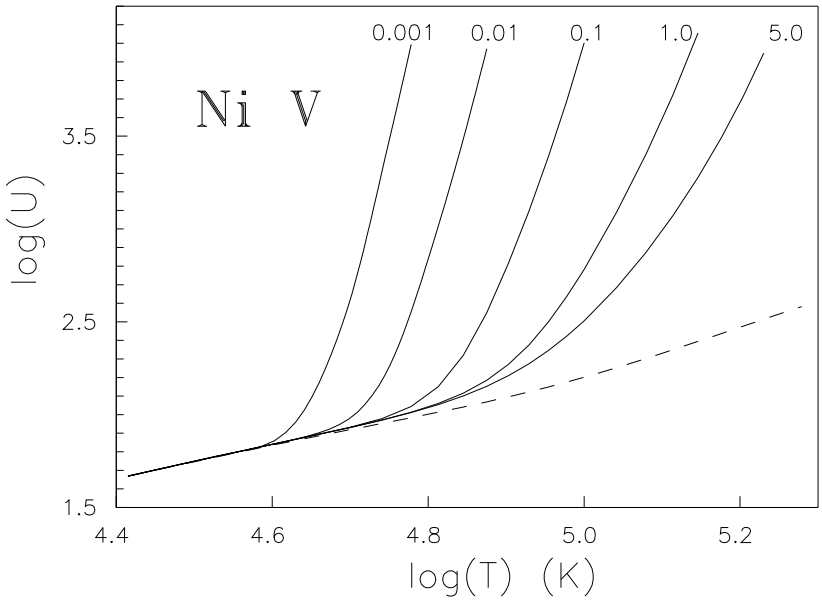

Fig. 1 : Run of partition functions of Ni V as function of gas temperature T and various parameters LIE. Solid lines represent our recommended results, whereas dashed line represents partition function computed from the observed levels only.

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REFERENCES

Drawin, H.W., and Felenbok, P. 1965, Data for Plasma in Local Thermodynamic Equilibrium (Gauthier-Villars, Paris)

Griem, H.R. 1964, Plasma Spectroscopy (McGraw-Hill Book Co., New York)

Halenka, J. 1988, Astron. Astrophys. Suppl., **75**, 47

Halenka, J. 1989, Astron. Astrophys. Suppl., **81**, 303

Halenka, J., and Grabowski, B. 1977, Astron. Astrophys., **54**, 757

Halenka, J., and Grabowski, B. 1984, Astron. Astrophys. Suppl., **57**, 43

Halenka, J., and Grabowski, B. 1986, Astron. Astrophys. Suppl., **64**, 495

Hubeny, I., and Lanz, T. 1992, Astron. Astrophys., **262**, 501

Hubeny, I., and Lanz, T. 1995, Astrophys. J, **439**, 875

Hummer, D.G., and Mihalas, D. 1988, Astrophys. J., **331**, 794

Irwin, A.W. 1981, Astrophys. J. Suppl., **45**, 621

Kurucz, R.L. 1994, CD-ROM No. 22

Madej, J., Halenka, J., and Grabowski, B. 1999, Astron. Astrophys., **343**, 531

Mihalas, D. 1978, Stellar Atmospheres (Freeman, San Francisco)

Traving, G., Baschek, B., and Holweger, H. 1966, Abh. Hamburger Sternw., **VIII**, No. 1

Table 1
Atomic partition functions for Ni V (decimal logarithms)

	Lowering of ionization energy (eV)								
T (K)	0.001	0.003	0.010	0.030	0.100	0.300	1.000	3.000	5.000
1000	1.0714	1.0714	1.0714	1.0714	1.0714	1.0714	1.0714	1.0714	1.0714
3000	1.2458	1.2458	1.2458	1.2458	1.2458	1.2458	1.2458	1.2458	1.2458
6000	1.3173	1.3173	1.3173	1.3173	1.3173	1.3173	1.3173	1.3173	1.3173
8000	1.3447	1.3447	1.3447	1.3447	1.3447	1.3447	1.3447	1.3447	1.3447
10000	1.3740	1.3740	1.3740	1.3740	1.3740	1.3740	1.3740	1.3740	1.3740
12000	1.4081	1.4081	1.4081	1.4081	1.4081	1.4081	1.4081	1.4081	1.4081
14000	1.4462	1.4462	1.4462	1.4462	1.4462	1.4462	1.4462	1.4462	1.4462
16000	1.4861	1.4861	1.4861	1.4861	1.4861	1.4861	1.4861	1.4861	1.4861
18000	1.5261	1.5261	1.5261	1.5261	1.5261	1.5261	1.5261	1.5261	1.5261
20000	1.5650	1.5650	1.5650	1.5650	1.5650	1.5650	1.5650	1.5650	1.5650
23000	1.6196	1.6196	1.6196	1.6196	1.6196	1.6196	1.6196	1.6196	1.6196
26000	1.6692	1.6692	1.6692	1.6692	1.6692	1.6692	1.6692	1.6692	1.6692
30000	1.7274	1.7274	1.7274	1.7274	1.7274	1.7274	1.7274	1.7274	1.7274
35000	1.7898	1.7894	1.7893	1.7893	1.7893	1.7893	1.7893	1.7893	1.7893
40000	1.8575	1.8448	1.8422	1.8418	1.8417	1.8417	1.8417	1.8417	1.8417
50000	2.6059	2.1647	1.9781	1.9395	1.9314	1.9302	1.9299	1.9298	1.9298
55000	3.3019	2.6546	2.1811	2.0193	1.9787	1.9721	1.9708	1.9704	1.9703
60000	3.9935	3.2352	2.5551	2.1802	2.0438	2.0181	2.0131	2.0115	2.0112
65000	4.7515	3.8183	3.0138	2.4548	2.1501	2.0756	2.0601	2.0551	2.0543
70000	5.6136	4.4428	3.4848	2.8054	2.3193	2.1551	2.1158	2.1030	2.1010
75000	6.5202	5.1417	3.9712	3.1802	2.5493	2.2667	2.1848	2.1571	2.1527
80000	7.4633	5.8866	4.4993	3.5634	2.8165	2.4143	2.2711	2.2188	2.2104
85000	8.4515	6.6585	5.0713	3.9642	3.0992	2.5924	2.3763	2.2890	2.2745
90000	9.4557	7.4630	5.6713	4.3931	3.3893	2.7901	2.4992	2.3680	2.3452
95000	10.4622	8.2918	6.2927	4.8493	3.6888	2.9978	2.6360	2.4553	2.4222
100000	11.4835	9.1284	6.9361	5.3258	4.0023	3.2103	2.7822	2.5501	2.5047
110000	13.5670	10.8261	8.2657	6.3273	4.6774	3.6474	3.0883	2.7565	2.6829
120000	15.6782	12.5674	9.6250	7.3798	5.4067	4.1113	3.4018	2.9781	2.8734
130000	17.7822	14.3359	11.0204	8.4622	6.1791	4.6108	3.7226	3.2103	3.0721
140000	19.8469	16.1070	12.4448	9.5740	6.9842	5.1464	4.0558	3.4522	3.2780
150000	21.8756	17.8536	13.8858	10.7152	7.8155	5.7149	4.4051	3.7054	3.4916
160000	23.8485	19.5773	15.3207	11.8792	8.6733	6.3124	4.7723	3.9711	3.7145
170000	25.7824	21.2664	16.7411	13.0523	9.5563	6.9356	5.1574	4.2504	3.9479
180000	27.6557	22.9208	18.1430	14.2208	10.4593	7.5829	5.5597	4.5434	4.1927
190000	29.4117	24.5349	19.5193	15.3780	11.3738	8.2518	5.9778	4.8495	4.4490
200000	31.0247	26.0761	20.8675	16.5179	12.2911	8.9376	6.4101	5.1677	4.7162
220000	33.8432	28.8464	23.4343	18.7264	14.1099	10.3366	7.3092	5.8338	5.2779
230000	35.0755	30.0715	24.6189	19.7872	15.0010	11.0389	7.7710	6.1777	5.5689
240000	36.2077	31.2000	25.7258	20.8097	15.8734	11.7375	8.2371	6.5258	5.8640
250000	37.2513	32.2417	26.7557	21.7855	16.7232	12.4292	8.7053	6.8760	6.1615
265000	38.6719	33.6610	28.1660	23.1506	17.9478	13.4466	9.4069	7.4012	6.6084
280000	39.9431	34.9316	29.4326	24.3949	19.1021	14.4319	10.1039	7.9219	7.0523
300000	41.4437	36.4318	30.9305	25.8789	20.5184	15.6831	11.0203	8.6033	7.6338
325000	43.0639	38.0519	32.5495	27.4908	22.0898	17.1285	12.1351	9.4278	8.3378
350000	44.4561	39.4440	33.9412	28.8797	23.4601	18.4309	13.2012	10.2180	9.0128
375000	45.6654	40.6533	35.1503	30.0874	24.6586	19.5929	14.2040	10.9714	9.6574
400000	46.7255	41.7134	36.2104	31.1469	25.7129	20.6271	15.1337	11.6861	10.2711
425000	47.6625	42.6505	37.1475	32.0837	26.6465	21.5491	15.9873	12.3606	10.8540
450000	48.4968	43.4847	37.9818	32.9178	27.4787	22.3743	16.7669	12.9940	11.4058
475000	49.2443	44.2323	38.7293	33.6652	28.2248	23.1160	17.4774	13.5861	11.9265
500000	49.9180	44.9060	39.4030	34.3389	28.8975	23.7859	18.1254	14.1380	12.4166
525000	50.5282	45.5163	40.0134	34.9492	29.5070	24.3936	18.7171	14.6513	12.8768
550000	51.0837	46.0717	40.5689	35.5047	30.0620	24.9472	19.2589	15.1282	13.3082
600000	52.0574	47.0455	41.5427	36.4785	31.0349	25.9187	20.2141	15.9831	14.0903
650000	52.8830	47.8711	42.3684	37.3043	31.8600	26.7430	21.0280	16.7235	14.7760
700000	53.5921	48.5802	43.0775	38.0134	32.5687	27.4513	21.7292	17.3683	15.3787
750000	54.2078	49.1959	43.6932	38.6292	33.1841	28.0666	22.3392	17.9336	15.9107
800000	54.7474	49.7355	44.2329	39.1689	33.7235	28.6059	22.8746	18.4325	16.3826
850000	55.2244	50.2125	44.7099	39.6459	34.2002	29.0826	23.3482	18.8756	16.8036
900000	55.6490	50.6371	45.1346	40.0706	34.6247	29.5071	23.7701	19.2717	17.1810
950000	56.0295	51.0176	45.5151	40.4511	35.0050	29.8875	24.1484	19.6277	17.5211
1000000	56.3723	51.3605	45.8580	40.7941	35.3478	30.2303	24.4895	19.9493	17.8290