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Atomic partition functions for chromium (*)

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Summary. — More realistic numerical values of the atomic partition functions, $U^{(r)}$, for CrI, CrII and CrIII are given for a wide range of the physical conditions of astrophysical and laboratory plasmas.

Key words : atomic partition functions — chromium — plasma.

1. Introduction.

In earlier papers of the authors (Halenka and Grabowski, 1977, 1984, hereafter Paper I and II, respectively) the general procedure of calculation of more realistic numerical values of the atomic partition functions (APF) has been described and applied to tin and iron. In the procedure, a simple cutoff approach to the lowering of the ionization energy (LIE) is maintained. The novelty consists in taking into account all the bound quantum states of a system under consideration (atom or ion), and among them the states above the « normal » continuum. Effect of these last, many-electron excitation states, on APF-values $U^{(r)}$ ($r = 0, 1, \ldots$, for neutral atom, single charged ion, etc.) is especially strong in the elements of low « normal » ionization energy and of complex energetic structure, as elements of the transition groups.

2. Calculations.

The aim of this paper is to obtain the realistic APF values for CrI, CrII and CrIII. We remind that the formalism used in Papers I and II demands preliminary calculations of $U^{(r+2)}$ and $U^{(r+1)}$ values in order to get the reliable $U^{(r)}$ ones. To the calculations, the values of the energetic levels of CrI-CrV (Moore, 1952; Ekberg, 1976; Sugar and Corlis, 1977; Ekberg and Engstrom, 1982) have been used; the levels of iron, magnesium and titanium served as comparative data. Thousand levels of chromium have been supplemented using approximation methods described in Papers I and II.

To calculate the numerical values of APF, the levels have been divided into groups as noted below (the symbols are the same as in Papers I and II) :

CrV : $\alpha^{(5)}$-*group* : the levels appearing in the aforementioned papers.

CrIV, CrIII, CrII and CrI : $\alpha^{(r)}$-*group* : sequences on the ground parent term of the configuration $3d^{(6-r)}$ [including the levels of the configuration $3d^{(7-r)}$ with proper coefficients of the fractional parentage, G_{1j}] and, furthermore, the sequence on the parent term $3d^4 4s(^6D)$, $\alpha'^{(1)}$.

$\beta^{(r)}$-*group* : sequences on the parent of the configuration $3d^{(6-r)}$ (except $\alpha^{(r)}$ sequence) [discrete summation over the levels of the configurations : $3d^{(6-r)}4s$, 4p, 4d and $3d^{(7-r)}$ (with coefficients G_{pj}, $p > 1$); the comparative sequence - $\alpha^{(r)}$] and, furthermore, the sequences on the parent terms of the configuration $3d^{(5-r)}4s$ for $r = 1, 2$ [discrete summation over the levels of the configurations : $3d^{(5-r)}4s^2$ and $3d^4 4s4p$ (for $r = 1$ only); the reference sequences - $\alpha^{(2)}$ and $\alpha'^{(1)}$ ones].

$\gamma^{(r)}$-*group* : remaining sequences [the reference sequence - $\alpha^{(r)}$]. The coefficients of the fractional parentage, G_{pj}, have been calculated according to Sobelman (1979).

3. Results and conclusions.

The $U^{(r)}$ values have been calculated in the temperature range 2000 K $\leqslant T \leqslant$ 40000 K, for LIE in the range 0.01 eV $\leqslant \Delta E^{(r)} \leqslant$ 2 eV. The APF values for CrI and CrII and CrIII are gathered in the tables (for CrI and CrII the temperature range is limited to that useful to applications; in higher temperatures the abundances of these ionization fractions are negligible). In the range 0.1 eV $\leqslant \Delta E^{(r)} \leqslant$ 2 eV the presented values of $U^{(r)}$ are equal or greater, and the ratios $U^{(r+1)}/U^{(r)}$ are equal or smaller as compared with corresponding values published earlier (e.g. Drawin and Felenbok, 1965; Irwin, 1981). The discrepancies of these quantities, taken properly from our tables and from above-mentioned papers, increase : (i) when $\Delta E^{(r)}$ decreases at T = const., and also (ii) when T increases at $\Delta E^{(r)}$ = const. The discrepancies have the same character as those shown in figure 2 in Paper II for iron.

In the present paper the range of the physical conditions for which the numerical values of APF are calculated, is

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substantially wider compared with that assumed by other authors — we have shifted the lower limit of LIE value, $\Delta E^{(r)}$, from 0.1 eV down to 0.01 eV. Qualitatively one can state that the previous calculation procedures just in here lead to $U^{(r)}$ values extremely different from suitable values presented in this paper.

The $\Delta E^{(r)}$ range from 0.1 down to 0.01 eV, as enlarged in this paper, corresponds to standard physical conditions in the stellar atmospheres and, partially, to laboratory arc plasma conditions. We expect that the effect of the more realistic APF values on the ionization balance, the equation of state, opacity, and stratification of the matter in the stellar atmospheres should be substantial. Details will be published elsewhere; for preliminary results see the papers by Grabowski and Halenka (1984); Halenka *et al.* (1984) on the effect under examination in iron and titanium plasmas.

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TABLE I. — *The atomic partition functions for CrI.*

T[K]	Lowering of the ionization energy [eV]					
	.01	.05	.10	.25	.50	1.00
2000	.7170E1	.7170E1	.7170E1	.7170E1	.7170E1	.7170E1
3000	.7731E1	.7731E1	.7731E1	.7731E1	.7731E1	.7731E1
4000	.8849E1	.8848E1	.8848E1	.8848E1	.8848E1	.8848E1
5000	.1053E2	.1050E2	.1049E2	.1049E2	.1049E2	.1049E2
5500	.1172E2	.1157E2	.1155E2	.1155E2	.1155E2	.1155E2
6000	.1339E2	.1286E2	.1282E2	.1280E2	.1280E2	.1279E2
6500	.1604E2	.1446E2	.1434E2	.1429E2	.1427E2	.1426E2
7000	.2062E2	.1649E2	.1619E2	.1606E2	.1602E2	.1599E2
7500	.2880E2	.1918E2	.1848E2	.1818E2	.1809E2	.1802E2
8000	.4334E2	.2283E2	.2135E2	.2073E2	.2054E2	.2040E2
8500	.6842E2	.2792E2	.2500E2	.2379E2	.2342E2	.2318E2
9000	.1102E3	.3510E2	.2971E2	.2749E2	.2683E2	.2639E2
9500	.1771E3	.4525E2	.3583E2	.3197E2	.3083E2	.3009E2
10000	.2806E3	.5954E2	.4381E2	.3741E2	.3553E2	.3435E2
10500	.4359E3	.7944E2	.5423E2	.4400E2	.4104E2	.3921E2
11000	.6628E3	.1068E3	.6775E2	.5201E2	.4748E2	.4475E2
11500	.9886E3	.1437E3	.8521E2	.6170E2	.5500E2	.5103E2
12000	.1452E4	.1931E3	.1076E3	.7341E2	.6376E2	.5812E2
12500	.2112E4	.2579E3	.1360E3	.8749E2	.7391E2	.6609E2
13000	.3060E4	.3422E3	.1717E3	.1044E3	.8565E2	.7503E2
13500	.4445E4	.4509E3	.2163E3	.1245E3	.9919E2	.8503E2
14000	.6511E4	.5901E3	.2716E3	.1483E3	.1147E3	.9616E2
14500	.9650E4	.7678E3	.3398E3	.1765E3	.1325E3	.1085E3
15000	.1448E5	.9944E3	.4235E3	.2096E3	.1528E3	.1222E3
16000	.3349E5	.1656E4	.6514E3	.2938E3	.2022E3	.1540E3
17000	.7805E5	.2756E4	.9926E3	.4081E3	.2654E3	.1925E3
18000	.1774E6	.4619E4	.1507E4	.5620E3	.3458E3	.2387E3
19000	.3862E6	.7801E4	.2288E4	.7687E3	.4474E3	.2940E3
20000	.7999E6	.1321E5	.3483E4	.1046E4	.5754E3	.3598E3
21000	.1581E7	.2227E5	.5311E4	.1419E4	.7362E3	.4379E3

TABLE II. — *The partition functions for CrII.*

T[K]	Lowering of the ionization energy [eV]					
	.01	.05	.10	.25	.50	1.00
2000	.6065E1	.6065E1	.6065E1	.6065E1	.6065E1	.6065E1
5000	.7180E1	.7180E1	.7180E1	.7180E1	.7180E1	.7180E1
8000	.1231E2	.1231E2	.1231E2	.1231E2	.1231E2	.1231E2
9000	.1519E2	.1518E2	.1518E2	.1518E2	.1518E2	.1518E2
10000	.1873E2	.1870E2	.1869E2	.1869E2	.1869E2	.1869E2
10500	.2079E2	.2070E2	.2069E2	.2069E2	.2069E2	.2069E2
11000	.2309E2	.2287E2	.2285E2	.2285E2	.2284E2	.2284E2
11500	.2571E2	.2522E2	.2518E2	.2517E2	.2516E2	.2516E2
12000	.2879E2	.2776E2	.2769E2	.2766E2	.2765E2	.2764E2
12500	.3253E2	.3051E2	.3038E2	.3032E2	.3030E2	.3029E2
13000	.3729E2	.3352E2	.3327E2	.3315E2	.3312E2	.3311E2
13500	.4355E2	.3682E2	.3638E2	.3616E2	.3611E2	.3609E2
14000	.5205E2	.4049E2	.3974E2	.3937E2	.3929E2	.3924E2
14500	.6379E2	.4463E2	.4339E2	.4278E2	.4264E2	.4257E2
15000	.8012E2	.4937E2	.4739E2	.4641E2	.4619E2	.4608E2
16000	.1342E3	.6139E2	.5672E2	.5443E2	.5392E2	.5367E2
17000	.2351E3	.7854E2	.6856E2	.6366E2	.6259E2	.6207E2
18000	.4146E3	.1038E3	.8409E2	.7446E2	.7238E2	.7138E2
19000	.7189E3	.1414E3	.1050E3	.8731E2	.8350E2	.8169E2
20000	.1214E4	.1971E3	.1337E3	.1028E3	.9626E2	.9316E2
21000	.1994E4	.2783E3	.1729E3	.1218E3	.1110E3	.1059E3
22000	.3206E4	.3945E3	.2263E3	.1453E3	.1282E3	.1203E3
23000	.5096E4	.5580E3	.2984E3	.1743E3	.1483E3	.1363E3
24000	.8111E4	.7846E3	.3947E3	.2103E3	.1719E3	.1544E3
25000	.1308E5	.1096E4	.5220E3	.2550E3	.1997E3	.1748E3
26000	.2156E5	.1523E4	.6888E3	.3101E3	.2325E3	.1979E3
27000	.3635E5	.2110E4	.9062E3	.3779E3	.2711E3	.2239E3
28000	.6241E5	.2924E4	.1189E4	.4612E3	.3166E3	.2533E3
29000	.1082E6	.4067E4	.1557E4	.5633E3	.3700E3	.2866E3
30000	.1874E6	.5693E4	.2039E4	.6881E3	.4327E3	.3243E3
31000	.3220E6	.8032E4	.2674E4	.8410E3	.5064E3	.3669E3
32000	.5467E6	.1142E5	.3515E4	.1026E4	.5926E3	.4151E3
33000	.9148E6	.1634E5	.4638E4	.1259E4	.6939E3	.4697E3
34000	.1509E7	.2347E5	.6145E4	.1542E4	.8126E3	.5314E3
35000	.2461E7	.3378E5	.8175E4	.1893E4	.9521E3	.6014E3

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TABLE III. — *The atomic partition functions for CrIII.*

T[K]	Lowering of the ionization energy [eV]					
	.05	.10	.25	.50	1.00	2.00
2000	.1961E2	.1961E2	.1961E2	.1961E2	.1961E2	.1961E2
8000	.2711E2	.2711E2	.2711E2	.2711E2	.2711E2	.2711E2
12000	.3592E2	.3592E2	.3592E2	.3592E2	.3592E2	.3592E2
14000	.4125E2	.4125E2	.4125E2	.4125E2	.4125E2	.4125E2
15000	.4405E2	.4405E2	.4405E2	.4405E2	.4405E2	.4405E2
16000	.4693E2	.4693E2	.4693E2	.4693E2	.4693E2	.4693E2
16500	.4840E2	.4840E2	.4840E2	.4840E2	.4840E2	.4840E2
17000	.4989E2	.4988E2	.4988E2	.4988E2	.4988E2	.4988E2
17500	.5139E2	.5138E2	.5138E2	.5138E2	.5138E2	.5138E2
18000	.5290E2	.5290E2	.5290E2	.5290E2	.5290E2	.5290E2
18500	.5444E2	.5443E2	.5442E2	.5442E2	.5442E2	.5442E2
19000	.5599E2	.5597E2	.5597E2	.5597E2	.5597E2	.5596E2
19500	.5756E2	.5754E2	.5753E2	.5752E2	.5752E2	.5752E2
20000	.5916E2	.5912E2	.5910E2	.5909E2	.5909E2	.5909E2
21000	.6244E2	.6234E2	.6230E2	.6228E2	.6228E2	.6228E2
22000	.6589E2	.6565E2	.6556E2	.6554E2	.6553E2	.6552E2
23000	.6959E2	.6911E2	.6892E2	.6887E2	.6885E2	.6884E2
24000	.7370E2	.7275E2	.7238E2	.7228E2	.7224E2	.7222E2
25000	.7842E2	.7666E2	.7598E2	.7579E2	.7573E2	.7569E2
26000	.8409E2	.8096E2	.7976E2	.7942E2	.7931E2	.7924E2
27000	.9114E2	.8582E2	.8377E2	.8320E2	.8301E2	.8289E2
28000	.1002E3	.9144E2	.8809E2	.8716E2	.8685E2	.8665E2
29000	.1120E3	.9811E2	.9281E2	.9134E2	.9085E2	.9054E2
30000	.1275E3	.1062E3	.9804E2	.9578E2	.9504E2	.9458E2
31000	.1481E3	.1161E3	.1039E3	.1006E3	.9945E2	.9877E2
32000	.1752E3	.1285E3	.1106E3	.1057E3	.1041E3	.1031E3
33000	.2107E3	.1438E3	.1184E3	.1114E3	.1091E3	.1077E3
34000	.2570E3	.1630E3	.1273E3	.1176E3	.1144E3	.1125E3
35000	.3166E3	.1870E3	.1379E3	.1245E3	.1201E3	.1176E3
36000	.3930E3	.2167E3	.1502E3	.1322E3	.1263E3	.1229E3
37000	.4901E3	.2535E3	.1648E3	.1408E3	.1331E3	.1285E3
38000	.6130E3	.2987E3	.1819E3	.1505E3	.1404E3	.1345E3
39000	.7680E3	.3542E3	.2021E3	.1615E3	.1484E3	.1409E3
40000	.9632E3	.4219E3	.2259E3	.1738E3	.1572E3	.1476E3

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