Wavelengths of Six Times Ionized Germanium, Ge VII

L. I. Podobedova[1,2] and A. N. Ryabtsev[2]
[1]*National Institute of Standards and Technology, Gaithersburg MD 20899 U.S.A.*
[2]*Institute of Spectroscopy RAS, Troitsk, 142092 Russia*

A compilation of Ge VII wavelengths has been carried out for the NIST Atomic Spectra Database on the World Wide Web. The compilation is based on our previous analyses of the germanium spectra: the $3d^8$-$3d^7 4p$ transition array in the range 160-210 Å, $3p^6 3d^8$-$3p^5 3d^9$ in the range 123-142 Å and $3d^7 4s$-$3d^7 4p$ in the range 739-987 Å [1-3] and the compilation of energy levels by Sugar and Musgrove [4]. A Russian publication [1] with the complete list of wavelengths of Ge VII is not well known; no new data on this spectrum were obtained since our analyses.

The Ge VII spectrum was excited in a three-electrode vacuum spark with the discharge parameters C=1-10 μF, L= 500-1000 nH, and U= 4-10 kV. Transitions to the ground state, lying in the region shorter than 200 Å, were studied from spectrograms obtained with a 3-m grazing incidence vacuum spectrograph (angle of incidence 85°) with a 3600 lines/mm grating. When working in the region longer than 700 Å, where transitions between excited states are located, we used a 6.65–m normal incidence vacuum spectrograph with a 1200 grooves/mm grating. The standard error for the wavelengths in the short-wave region was estimated at 0.004 Å, and in the long-wavelength region, 0.007 Å.

The Ge VII spectrum belongs to the iron isoelectronic sequence, having a ground-state configuration $3p^6 3d^8$ and the lowly excited configurations $3d^7 4s$, $3d^7 4p$, $3p^5 3d^9$ and $3d^7 4f$. The $3p^5 3d^9$ configuration, with the excitation of an electron from an inner shell, which is unknown at the beginning of the isoelectronic sequence, decreases in energy with respect to valence electron excitations as the ionization stage increases. As a result, a strong interaction between the $3p^6 3d^7 4p$ and $3p^5 3d^9$ configurations is observed for a number of ions of the sequence including Ge VII (Fig. 1). The analysis of the resonance transition array $3d^8$ - $3d^7 4p$, located in the region 160-210 Å, has been carried out in [2]. All levels of the ground configuration $3d^8$ and 85 of 110 levels of the $3d^7 4p$ configuration have been found. Other levels of the latter configuration either do not have transitions to the ground configuration or the transitions are very week. These levels can be found by studying transitions to the $3d^7 4s$ configuration. The analysis of the $3d^7 4p$-$3d^7 4s$ and $3p^6 3d^8$-$3p^5 3d^9$ transition arrays and the necessary corrections of the $3d^7 4p$ configuration were made in our subsequent work [3]. Thus all levels of the $3d^8$, $3d^7 4s$, $3s^7 4p$ and $3p^5 3d^9$ configurations were established. Later, these levels were compiled in [4].

The purpose of the present work is to check our previous analysis and to present a wavelength table in the format of the NIST Database. It should be noted that we interpreted the spectra on the basis of single-configuration calculations because of our calculation limitations at that time. Besides, the knowledge of other ions of the Fe-like isoelectronic sequence was very poor. In 1980, when we started to work on the Ge VII spectrum, the highest well-studied member of this sequence was Cu IV. The spectra Zn V and Ga VI were under study, and only preliminary values for the levels of the term $3d^8\ ^3F$ were known. Since that time, a great amount of work has been done for many spectra of Fe-like ions. Now, the resonance transition array $3d^8$-$3d^7 4p$ has also been studied for the Zn V-Br X, Rb XII and Sr XIII ions. The $3p^6 3d^8$-$3p^5 3d^9$ transition array is known for the Ga VI-Br X and Ag XXII-Sn XXV ions. In these latter ions, this transition array becomes resonant. The transition array between the excited configurations $3d^7 4p$ and $3d^7 4s$ has been analyzed in the Zn V-Ge VII and Br X ions.

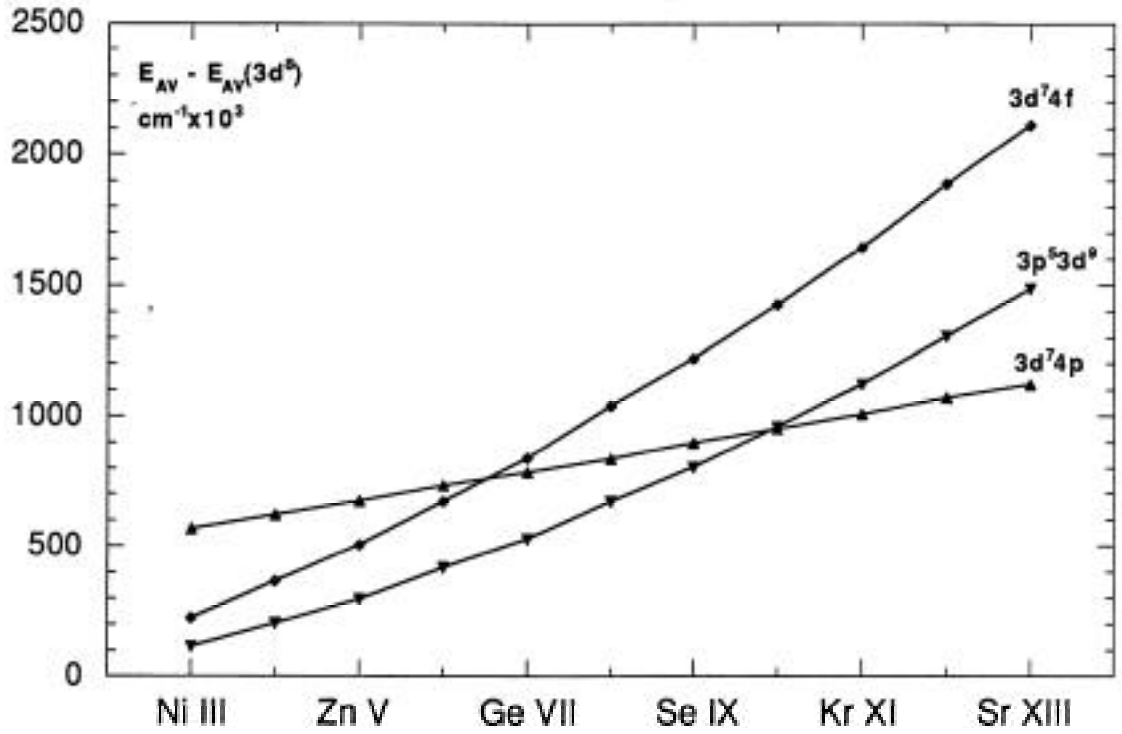

Figure 1: Average energies of the three lowest odd configurations realtive to that of the ground configuration along the Fe I sequence.

The Hartree-Fock (HF) and least–square fit (LSF) calculations were carried out for the studied configurations by means of the Cowan code. The final values of the corresponding parameters and their ratios are given in Table 1. All 47 energy levels of the even $3d^8$ and $3d^74s$ configurations are included in the LSF calculation, and the mean-square deviation σ is 91cm^{-1}. The effective parameters β and T for the $3d^8$ configuration were fixed because of the instability of the fitting process, and the values for them were taken to be the same as for the $3d^74s$ configuration. The odd configurations $3d^74p$, $3p^53d^9$ and $3d^74f$ were included in the calculation with their interaction. As noted above, there is a strong interaction between the $3d^74p$ and $3p^53d^9$ configurations, even though the average energies of these configurations are separated by 226,640 cm^{-1}. According to the HF calculation, the $3d^74f$ configuration is located 83,680 cm^{-1} higher and also disturbs some levels of the $3p^53d^9$ configuration. All 122 energy levels of the $3d^74p$ and $3p^53d^9$ configurations were included in the LSF calculation and the mean square deviation σ is 131 cm^{-1}. We increased the average energy of the unknown $3d^34f$ configuration by 3005 cm^{-1} with respect to the HF value as in the $3d^74p$ configuration. All parameters were fixed according to the usual scaling factors from the HF values: 0.85 for the electrostatic interaction and unity for the spin-orbit interaction. The configuration interaction parameters were scaled by a factor of 0.85 for both even and odd configurations. In conclusion, we note that the LSF/HF ratios for all studied configurations are close to those predicted by extrapolation along the isoelectronic series. It is also interesting to note that the $3p^53d^9\ {}^1F_3^\circ$ level deviates from the computed value by only -7 cm^{-1}; in the single-configuration calculation [1] this deviation was -7155 cm^{-1}.

On the basis of this work, we confirm our previous classifications for all spectral lines and energy levels except for the $3p^63d^8\ {}^3P_1$-$3p^53d^9\ {}^3P_0^\circ$ transition. Instead of the line at 135.018 Å, the correct line is at 135.008 Å. Correspondingly, the $3p^53d^9\ {}^3P_0^\circ$ level, having only one transition to the ground state, changes from 769854 cm^{-1} to 769908 cm^{-1}. We also added second classifications for three lines, in accordance with the transition probabilities calculated with the final

parameters of the LSF calculation. Besides, a few misprints in the designations of the classified lines have been corrected. After checking the analysis, we prepared a table of the classified wavelengths including more than 520 Ge VII spectral lines. This table will appear in an upcoming new version of the NIST Atomic Spectra Database.

References

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Table 1: Parametric values of the energy integrals and their ratios to the Hartree-Fock values for the 3d8 +3d7 4s and 3d7 4p + 3p5 3d9 + 3d7 4f configurations in GeVII (cm^{-1}).

Configuration	Parameter	LSF		Error	HF	LSF/HF*
3p6 3d8	Eav(3d8)	19212		40	21541	-2329
	F2(3d,3d)	130539		311	148806	0.877
	F4(3d,3d)	83108		283	93874	0.885
	α(3d)	66		007		
	β(3d)	550	f			
	T(3d)	-8	f			
	ζ(3d)	1948		43	1950	0.999
3d7 4s	Eav(3d7 4s)	436151		19	434305	1846
	F2(3d,3d)	134696		104	154339	0.873
	F4(3d,3d)	87076		203	97613	0.892
	α(3d)	68		7		
	β(3d)	550		121		
	T(3d)	-8		1		
	ζ(3d)	2107		18	2069	1.018
	G2(3d,4s)	14097		82	14281	0.987
	R2(3d,3d;3d,4s)	11270	f		13259	0.850
	σ	91				
3d7 4p	Eav(3d7 4p)	553079		15	550074	3005
	F2(3d,3d)	135781		89	154506	0.879
	F4(3d,3d)	87292		193	97730	0.893
	α	57		6		
	β	768		100		
	T(3d)	-9		1		
	ζ(3d)	2092		16	2072	1.010
	ζ(4p)	3812		34	3278	1.163
	F2(3d,4p)	35302		129	36020	0.980
	G1(3d,4p)	11210		58	11938	0.939
	G3(3d,4p)	11284		151	11409	0.989
3p5 3d9	Eav(3p5 3d9)	779719		57	807033	-27314
	ζ(3p)	23397		124	22166	1.056
	ζ(3d)	1857		62	1946	0.954
	F1(3p,3d)	11686		627		
	F2(3p,3d)	148729		548	149744	0.993
	G1(3p,3d)	148827		362	181099	0.822
	G2(3p,3d)	-5981		698		
	G3(3p,3d)	114830		594	112606	1.020
3d7 4f	Eav(3d7 4f)	863400	f		860395	3005
	F2(3d,3d)	131967	f		155255	0.850
	F4(3d,3d)	83502	f		98238	0.850
	ζ(3d)	2087	f		2087	1.000
	ζ(4f)	8	f		8	1.000
	F2(3d,4f)	12868	f		15139	0.850
	F4(3d,4f)	4711	f		5542	0.850
	G1(3d,4f)	5841	f		6872	0.850
	G3(3d,4f)	3365	f		3959	0.850
	G5(3d,4f)	2309	f		2717	0.850
	R1(3d,4p;3d,3d)	12652	f		14885	0.850
	R3(3d,4p;3d,3d)	12651	f		14883	0.850
	R2(3d,4p;3d,4f)	13408	f		15774	0.850
	R4(3d,4p;3d,4f)	4586	f		5395	0.850
	R1(3d,4p;4f,3d)	1655	f		1947	0.850
	R3(3d,4p;4f,3d)	1694	f		1993	0.850
	R1(3d,3d;3d,4f)	-25658	f		-30185	0.850
	R3(3d,3d;3d,4f)	-13185	f		-15512	0.850
	σ	131				

* Differences Eav(LSF)-Eav(HF) are presented for Eav. f - The parameters are fixed.