Chapter 11

Atomic physics

	page
Atomic physics	256
Spectroscopic terminology	256
Emission and absorption of radiation	256
X-ray atomic energy levels	258
X-ray energy level diagram	261
X-ray wavelengths	262
Wavelengths of K series lines	262
Wavelengths of the more prominent L group lines	264
Bibliography	265

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Spectroscopic terminology

Orbital angular momentum L or l	0	1	2	3	4	5	6	7	8
L	S	P	D	F	G	H	I	K	L
l	s	p	d	f	g	h	i	k	l

$L = \sum l$ (individual electrons), orbital angular momentum,
$S = \sum s$ (individual electrons), spin angular momentum,
$J = L + S$ (LS coupling), total angular momentum,
$J = \sum j$; $j = l + s$ (jj coupling),
M = magnetic quantum number; components of J in magnetic field.

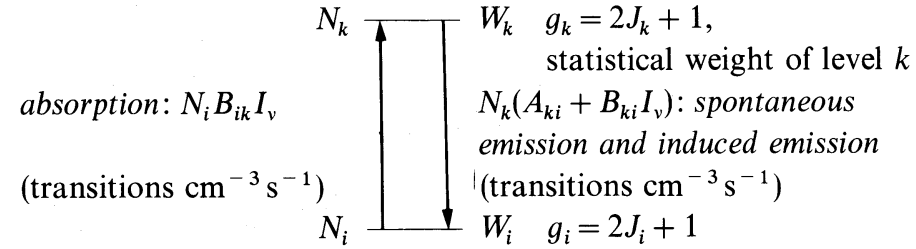
n (total quantum number)	1	2	3	4	5	6	7
Shell	K	L	M	N	O	P	Q

The quantities n, l, S, L, J, M define a Zeeman *state*.
The quantities n, l, S, L, J define a *level* which includes $2J + 1$ *states*, e.g., the atomic level $2p^3\ {}^4S^0_{3/2}$.
Interpretation:

- 2: outer electrons, $n = 2$ (L shell).
- p^3: 3 outer electrons, $l = 1$.
- 4: multiplicity = 4 ($2S + 1 = 4$, $S = 3/2$, the spin).
- S: orbital momentum $L = 0$.
- 3/2: $J = 3/2$.
- 0: the level has odd parity.

The quantities n, l, S, L define an atomic *term*, the set of $(2S + 1) \times (2L + 1)$ states characterized by given values of L and S.
A transition between two *levels* is called a spectral *line*.
The totality of transitions between two *terms* is a *multiplet*.

Emission and absorption of radiation (cgs units)



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where

A_{ki} = Einstein coefficient of spontaneous emission,
N_k = number of atoms per unit volume in level k,
B_{ik} = induced transition probability from level i to level k,
I_ν = specific intensity of radiation field at frequency ν,
$h\nu = W_k - W_i$, transition energy.

$$g_k B_{ki} = g_i B_{ik},$$

$$\frac{g_k}{g_i} A_{ki} = \frac{2h\nu^3}{c^2} B_{ik} = \frac{8\pi^2 e^2 \nu^2}{mc^3} f_{ik},$$

where f_{ik} = absorption oscillator strength.

$$\sigma_i = \int \sigma_\nu \, d\nu = \frac{\pi e^2}{mc} f_{ik} N_i, \text{ is the}$$

integrated atomic scattering coefficient for a spectrum line.
σ_ν = atomic scattering coefficient near an absorption line.

Thermal equilibrium

$$\frac{N_k}{N_i} = \frac{g_k}{g_i} e^{-(W_k - W_i)/kT} \quad \text{(Boltzmann's formula).}$$

Doppler shift

$$\Delta\lambda/\lambda \approx v/c \quad (v = \text{velocity of source}).$$

Doppler width of spectral line (FWHM, Maxwellian distribution)

$$\frac{\Delta\lambda_D}{\lambda} = \frac{2[(2\ln 2)kT/M]^{1/2}}{c} = 7.162 \times 10^{-7} \sqrt{\left[\frac{T\,(\mathrm{K})}{\text{at. wt.}}\right]},$$

where M is the mass of the radiating atom.

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X-ray atomic energy levels (eV)

Z	element	K	L_I	$L_{II,III}$
1	H	13.598		
2	He	24.587		
3	Li	54.75		
4	Be	111.0		
5	B	188.0		4.7
6	C	283.8		6.4
7	N	401.6		9.2
8	O	532.0	23.7	7.1
9	F	685.4	31	8.6
10	Ne	866.9	45	18.3
11	Na	1072.1	63.3	31.1
12	Mg	1305.0	89.4	51.4
13	Al	1559.6	117.7	73.1
14	Si	1838.9	148.7	99.2
15	P	2145.5	189.3	132.2
16	S	2472.0	229.2	164.8

Z	element	K	L_I	L_{II}	L_{III}	M_I	$M_{II,III}$	$M_{IV,V}$
17	Cl	2822.4	270.2	201.6	200.0	17.5	6.8	
18	Ar	3202.9	320.	247.3	245.2	25.3	12.4	
19	K	3607.4	377.1	296.3	293.6	33.9	17.8	
20	Ca	4038.1	437.8	350.0	346.4	43.7	25.4	
21	Sc	4492.8	500.4	406.7	402.2	53.8	32.3	6.6
22	Ti	4966.4	563.7	461.5	455.5	60.3	34.6	3.7
23	V	5465.1	628.2	520.5	512.9	66.5	37.8	2.2
24	Cr	5989.2	694.6	583.7	574.5	74.1	42.5	2.3
25	Mn	6539.0	769.0	651.4	640.3	83.9	48.6	3.3
26	Fe	7112.0	846.1	721.1	708.1	92.9	54.0	3.6

Permitted transitions

K series	*L* series
$K\alpha_1 = K - L_{III}$	$L\alpha_1 = L_{III} - M_V$
$K\alpha_2 = K - L_{II}$	$L\alpha_2 = L_{III} - M_{IV}$
$K\beta_1 = K - M_{III}$	$L\beta_1 = L_{II} - M_{IV}$
$K\beta_3 = K - M_{II}$	
$K\beta_2 = K - N_{II,III}$	

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Z	element	K	L_I	L_{II}	L_{III}	M_I	M_{II}	M_{III}	$M_{IV,V}$
27	Co	7708.9	925.6	793.6	778.6	100.7	59.5	2.9	
28	Ni	8332.8	1008.1	871.9	854.7	111.8	68.1	3.6	
29	Cu	8978.9	1096.6	951.0	931.1	119.8	73.6	1.6	
30	Zn	9658.6	1193.6	1042.8	1019.7	135.9	86.6	8.1	
31	Ga	10 367.1	1297.7	1142.3	1115.4	158.1	106.8	102.9	17.4
32	Ge	11 103.1	1414.3	1247.8	1216.7	180.0	127.9	120.8	28.7

Z	element	K	L_I	L_{II}	L_{III}	M_I	M_{II}	M_{III}	M_{IV}	M_V	N_I	N_{II}	N_{III}
47	Ag	25 514.0	3805.8	3523.7	3351.1	717.5	602.4	571.4	372.8	366.7	95.2	62.6	55.9
53	I	33 169.4	5188.1	4852.1	4557.1	1072.1	930.5	874.6	631.3	619.4	186.4	122.7	
54	Xe	34 561.4	5452.8	5103.7	4782.2		999.0	937.0		672.3		146.7	
55	Ca	35 984.6	5714.3	5359.4	5011.9	1217.1	1065.0	997.6	739.5	725.5	230.8	172.3	161.6
74	W	69 525.0	12 099.8	11 544.0	10 206.8	2819.6	2574.9	2281.0	1871.6	1809.2	595.0	491.6	425.3
78	Pt	78 394.8	13 879.9	13 272.6	11 563.7	3296.0	3026.5	2645.4	2201.9	2121.6	722.0	609.2	519.0
79	Au	80 724.9	14 352.8	13 733.6	11 918.7	3424.9	3147.8	2743.0	2291.1	2205.7	758.8	643.7	545.4
82	Pb	88 004.5	15 860.8	15 200.0	13 035.2	3850.7	3554.2	3066.4	2585.6	2484.0	893.6	763.9	644.5
92	U	115 606.1	21757.4	20 947.6	17 166.3	5548.0	5182.2	4303.4	3727.6	3551.7	1440.8	1272.6	1044.9

Z	element	N_{IV}	N_V	N_{VI}	N_{VII}	O_I	O_{II}	O_{III}	O_{IV}	O_V	P_I	P_{II}	P_{III}
47	Ag	3.3											
53	I	49.6				13.6							
54	Xe							3.3					
55	Ca	78.8	76.5			22.7	13.1	11.4					
74	W	258.8	245.4	36.5	33.6	77.1	46.8	35.6	6.1				
78	Pt	330.8	313.3	74.3	71.1	101.7	65.3	51.7	2.2				
79	Au	352.0	333.9	86.4	82.8	107.8	71.7	53.7	2.5				
82	Pb	435.2	412.9	142.9	138.1	147.3	104.8	86.0	21.8	19.2	3.1	0.7	
92	U	780.4	737.7	391.3	380.9	323.7	259.3	195.1	105.0	96.3	70.7	42.3	32.3

(List from Bearden, J. A. and Burr, A. F., *Rev. Mod. Phys.*, **39**, 125, 1967.)

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X-ray atomic energy levels (*cont.*)

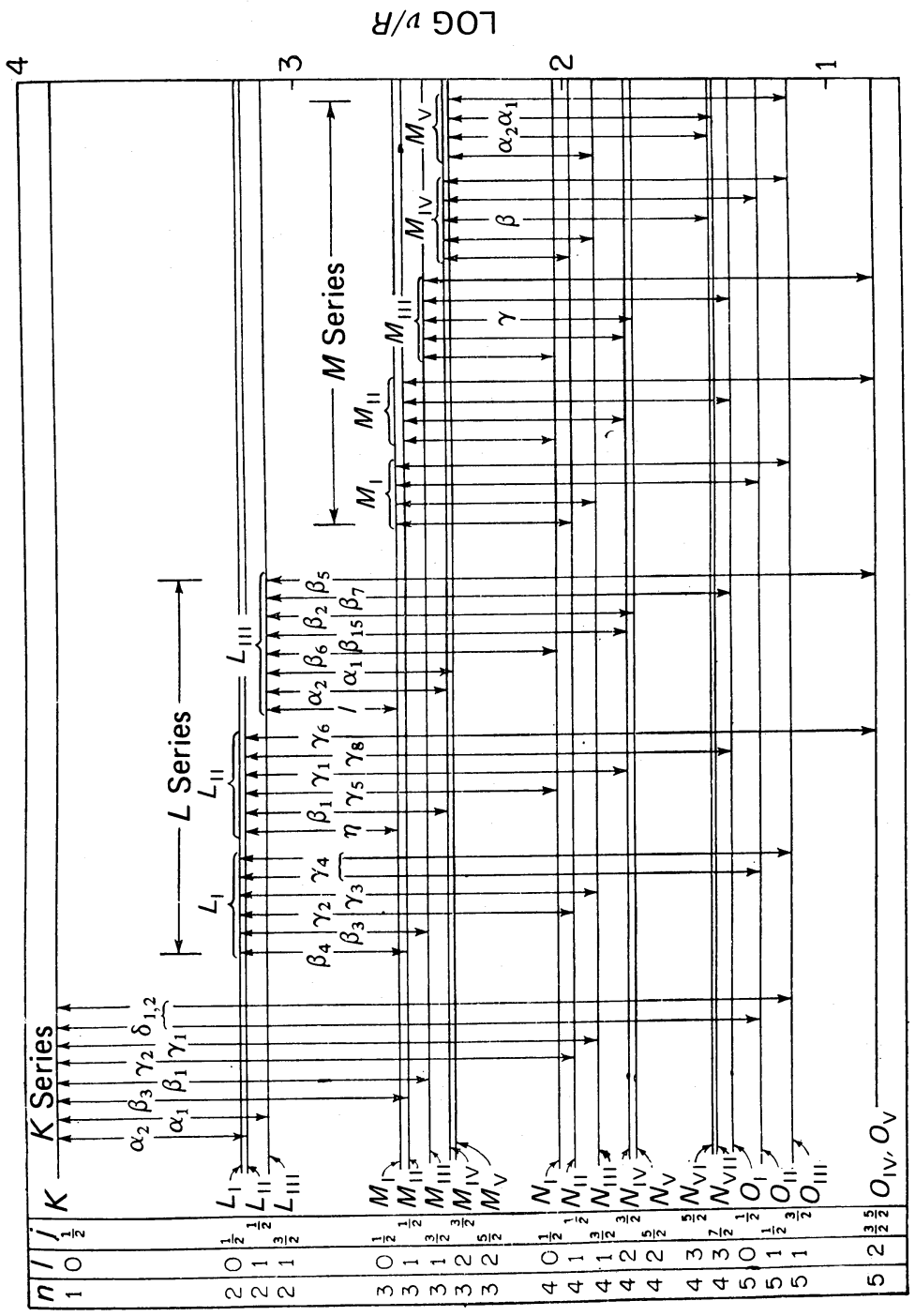
Notation for X-ray lines

Siegbahn notation	Transition	Siegbahn notation	Transition	Siegbahn notation	Transition	Siegbahn notation	Transition
$K\alpha_1$	KL_{III}	$L\gamma_2$	L_IN_{II}	LV	$L_{II}N_{VI}$	$L\beta_2$	$L_{III}N_V$
$K\alpha_2$	KL_{II}	$L\gamma_3$	L_IN_{III}	$L\gamma_8$	$L_{II}O_I$	Lu	$L_{III}N_{VI,VII}$
$K\beta_3$	KM_{II}	$L\gamma_{11}$	L_IN_V	$L\gamma_6$	$L_{II}O_{IV}$	$L\beta_7$	$L_{III}O_I$
$K\beta_1$	KM_{III}	$L\gamma_4$	L_IO_{III}	Ll	$L_{III}M_I$	$L\beta_3$	$L_{III}O_{IV,V}$
$K\beta_5$	$KM_{IV,V}$	$L\gamma_{13}$	$L_IP_{II,III}$	Lt	$L_{III}M_{II}$	$M\gamma$	$M_{III}N_V$
$K\beta_2$	$KN_{II,III}$	$L\eta$	$L_{II}M_I$	Ls	$L_{III}M_{III}$	$M\beta$	$M_{IV}N_{VI}$
$K\beta_4$	$KN_{IV,V}$	$L\beta_{17}$	$L_{II}M_{III}$	$L\alpha_2$	$L_{III}M_{IV}$	$M\zeta_2$	$M_{IV}N_{II}$
$L\beta_4$	L_IM_{II}	$L\beta_1$	$L_{II}M_{IV}$	$L\alpha_1$	$L_{III}M_V$	$M\zeta_1$	$M_{IV}N_{III}$
$L\beta_3$	L_IM_{III}	$L\gamma_5$	$L_{II}N_I$	$L\beta_6$	$L_{III}N_I$	$M\alpha_2$	M_VN_{VII}
$L\beta_{10}$	L_IM_{IV}	$L\gamma_1$	$L_{II}N_{IV}$	$L\beta_{13}$	$L_{III}N_{IV}$	$M\alpha_1$	M_VN_{VII}
$L\beta_9$	L_IM_V						

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X-ray energy level diagram

X-ray energy-level diagram for ^{92}U, showing the transitions permitted by the selection rules $\Delta l = \pm 1$; $\Delta j = \pm 1, 0$. (Adapted from Richtmyer, F. K., Kennard, E. H. & Lauritsen, T., *Introduction to Modern Physics*, McGraw-Hill Book Company, 1955.)



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X-ray wavelengths

Wavelengths of K series lines representing transitions in the ordinary X-ray energy-level diagram allowed by the selection principles (Ångstrom)

Siegbahn		$K\alpha_2$	$K\alpha_1$	$K\beta$	$K\beta_1$	$K\beta_2$
Sommerfeld		$K\alpha'$	$K\alpha$	$K\beta_2$	$K\beta$	$K\gamma$
transition		K–L_{II}	K–L_{III}	K–M_{II}	K–M_{III}	K–$L_{II}N_{III}$
4	Be	115.7				
5	B	67.71				
6	C	44.54				
7	N	31.557				
8	O	23.567				
9	F	18.275				
11	Na	11.885		11.594		
12	Mg	9.869		9.539		
13	Al	8.3205		7.965		
14	Si	7.111 06		6.7545		
15	P	6.1425		5.7921		
16	S	5.3637	5.3613	5.0211		
17	Cl	4.7212	4.7182	4.3942		
19	K	3.737 07	3.733 68	3.4468		
20	Ca	3.354 95	3.351 69	3.0834		
21	Sc	3.028 40	3.025 03	2.7739		
22	Ti	2.746 81	2.743 17	2.5090		
23	V	2.502 13	2.498 35	2.2797		
24	Cr	2.288 91	2.285 03	2.0806		
25	Mn	2.101 49	2.097 51	1.906 20		
26	Fe	1.936 012	1.932 076	1.753 013		
27	Co	1.789 19	1.785 29	1.617 44		
28	Ni	1.658 35	1.654 50	1.479 05		1.485 61
29	Cu	1.541 232	1.537 395	1.389 35		1.378 24
30	Zn	1.436 03	1.432 17	1.292 55		1.281 07
31	Ga	1.340 87	1.337 15	1.205 20		1.1938
32	Ge	1.255 21	1.251 30	1.126 71		1.114 59
33	As	1.177 43	1.173 44	1.055 10		1.042 81
34	Se	1.106 52	1.102 48	0.990 13		0.977 91
35	Br	1.041 66	1.037 59	0.930 87		0.918 53
36	Kr	0.9821	0.9781	0.8767		0.8643
37	Rb	0.927 76	0.923 64	0.827 49	0.826 96	0.814 76
38	Sr	0.877 61	0.873 45	0.781 83	0.781 30	0.769 21
39	Y	0.831 32	0.827 12	0.739 72	0.739 19	0.727 13
40	Zr	0.788 51	0.784 30	0.700 83	0.700 28	0.688 50
41	Nb	0.748 89	0.744 65	0.664 96	0.664 38	0.652 80
42	Mo	0.712 105	0.707 831	0.631 543	0.630 978	0.619 698
43	Te	0.675	0.672	0.601		
44	Ru	0.646 06	0.641 74	0.571 93	0.571 31	0.560 51
45	Rh	0.616 37	0.612 02	0.545 09	0.544 49	0.533 96
46	Pd	0.588 63	0.584 27	0.520 09	0.519 47	0.509 18
47	Ag	0.562 67	0.558 28	0.496 65	0.496 01	0.486 03

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Wavelengths of K series lines representing transitions in the ordinary X-ray energy-level diagram allowed by the selection principles (*cont.*)

Siegbahn Sommerfeld transition	$K\alpha_2$ $K\alpha'$ $K-L_{II}$	$K\alpha_1$ $K\alpha$ $K-L_{III}$	$K\beta$ $K\beta_2$ $K-M_{II}$	$K\beta_1$ $K\beta$ $K-M_{III}$	$K\beta_2$ $K\gamma$ $K-L_{II}N_{III}$
48 Cd	0.538 32	0.533 90	0.474 71	0.474 08	0.464 20
49 In	0.515 48	0.511 06	0.454 23	0.453 58	0.444 08
50 Sn	0.494 02	0.489 57	0.434 95	0.434 30	0.424 99
51 Sb	0.473 87	0.469 31		0.416 23	0.407 10
52 Te	0.454 91	0.450 37		0.399 26	0.390 37
53 I	0.437 03	0.432 49	0.382 92	0.383 15	0.374 71
54 Xe	0.417			0.360	
55 Cs	0.404 11	0.399 59	0.354 36	0.353 60	0.345 16
56 Ba	0.388 99	0.384 43	0.340 89	0.340 22	0.332 22
57 La	0.374 66	0.370 04	0.328 09	0.327 26	0.319 66
58 Ce	0.361 10	0.356 47	0.315 72	0.315 01	0.307 70
59 Pr	0.348 05	0.343 40	0.304 39	0.303 60	0.296 25
60 Nd	0.335 95	0.331 25	0.293 51	0.292 75	0.285 73
62 Sm	0.313 02	0.308 33	0.273 25	0.272 50	0.265 75
63 Eu	0.302 65	0.297 90	0.263 86	0.263 07	0.256 45
64 Gd	0.292 61	0.287 82	0.254 71	0.253 94	0.247 62
65 Tb	0.282 86	0.278 20	0.246 29	0.245 51	0.239 12
66 Dy	0.273 75	0.269 03	0.237 87	0.237 10	0.231 28
67 Ho	0.264 99	0.260 30			
68 Er	0.256 64	0.251 97	0.223 00	0.222 15	0.216 71
69 Tm	0.248 61	0.243 87	0.215 58	0.214 87	
70 Yb	0.240 98	0.230 28	0.209 16	0.208 34	0.203 22
71 Lu	0.233 58	0.2282	0.202 52	0.201 71	0.196 49
72 Hf	0.226 53	0.221 73	0.195 83	0.195 15	0.190 42
73 Ta	0.219 73	0.214 88		0.189 91	0.184 52
74 W	0.213 37	0.208 56	0.184 75	0.183 97	0.179 06
76 Os	0.201 31	0.196 45		0.173 61	0.168 75
77 Ir	0.195 50	0.190 65		0.168 50	0.163 76
78 Pt	0.190 04	0.182 23		0.163 70	0.158 87
79 Au	0.184 83	0.179 96		0.159 02	0.154 26
81 Tl	0.174 66	0.169 80		0.150 11	0.145 39
82 Pb	0.170 04	0.165 16		0.146 06	0.141 25
83 Bi	0.165 25	0.160 41		0.142 05	0.136 21
92 U	0.130 95	0.126 40		0.111 87	0.108 42

(From *Smithsonian Physical Tables.*)

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Wavelengths of the more prominent L group lines (Ångstrom)

Siegbahn		α_2	α_1	β_1	l	η	β_2	γ_1
Sommerfeld		α'	α	β	ε	η	γ	δ
transition		L_{III}–M_{IV}	L_{III}–M_V	L_{II}–M_V	L_{III}–M_I	L_{II}–M_I	L_{III}–N_V	L_{II}–N_{IV}
16	S		...	...	83.75			
20	Ca		36.27	...	40.90			
21	Sc		31.37	...	35.71			
22	Ti		27.37	...	31.33			
23	V		24.31	...	27.70			
24	Cr		21.53	21.19	23.84	23.28		
25	Mn		19.40	19.04	22.34			
26	Fe		17.57	17.23	20.09	19.76		
27	Co		15.93	15.63	18.25	17.86		
28	Ni		14.53	14.25	16.66	16.28		
29	Cu		13.306	13.027	15.26	14.87		
30	Zn		12.229	11.960	13.97	13.61		
31	Ga		11.27	11.01	12.89	12.56		
32	Ge		10.415	10.153	11.922	11.587		
33	As		9.652	9.395	11.048	10.711		
34	Se		8.972	8.718	10.272	9.939		
35	Br		8.358	8.109	9.564	9.235		
37	Rb		7.3027					
38	Sr		6.8486	6.610	7.822	7.506		
39	Y		6.4357	6.2039	...	7.0310		
40	Zr		6.057	5.8236	5.5742	5.3738		
41	Nb	5.718	5.7120	5.4803	5.2260	5.0248		
42	Mo	5.401	5.3950	5.1665	4.9100			
44	Ru	4.8437	4.8357	4.6110	4.3619	4.1728		
45	Rh	4.5956	4.5878	4.3640	4.1221	3.9357		
46	Pd	4.3666	4.3585	4.1373	3.9007	3.7164		
47	Ag	4.1538	4.1456	3.9266	3.6938	3.5149		
48	Cd	3.9564	3.9478	3.7301	3.5064	3.3280		
49	In	3.7724	3.7637	3.5478	3.3312	3.1553		
50	Sn	3.601 51	3.592 57	3.3779	3.168 61	2.994 94		
51	Sb	3.4408	3.4318	3.2184	3.0166	2.8451		
52	Te	3.2910	3.2820	3.0700	2.8761	2.7065		
53	I	3.1509	3.1417	2.9309	2.7461	2.5775		
55	Cs	2.8956	2.8861	2.6778	2.5064	2.3425		
56	Ba	2.7790	2.7696	2.5622	2.3993	2.2366		
57	La	2.6689	2.6597	2.4533	2.2980	2.1372		
58	Ce	2.5651	2.5560	2.3510	2.2041	2.0443		
59	Pr	2.4676	2.4577	2.2539	2.1148	1.9568		
60	Nd	2.3756	2.3653	2.1622	2.0314	1.8738		
62	Sm	2.2057	2.1950	1.9936	1.8781	1.7231		
63	Eu	2.1273	2.1163	1.9163	1.8082	1.6543		

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Wavelengths of the more prominent L group lines (*cont.*)

Siegbahn Sommerfeld transition	α_2 α' L_{III}–M_{IV}	α_1 α L_{III}–M_V	β_1 β L_{II}–M_V	l ε L_{III}–M_I	η η L_{II}–M_I
64 Gd	2.0526	2.0419	1.8425	1.7419	1.5886
65 Tb	1.9823	1.9715	1.7727	1.6790	1.5266
66 Dy	1.9156	1.9046	1.7066	1.6198	1.4697
67 Ho	1.8521	1.8410	1.6435	1.5637	1.4142
68 Er	1.792 02	1.780 68	1.584 09	1.510 94	1.3611
69 Tm	1.7339	1.7228	1.5268	1.4602	1.3127
70 Yb	1.679 42	1.668 44	1.4725	1.412 61	1.265 12
71 Lu	1.6270	1.616 17	1.420 67	1.367 31	1.219 74
72 Hf	1.577 04	1.566 07	1.3711	1.3235	1.1765
73 Ta	1.529 78	1.518 85	1.324 23	1.281 90	1.135 58
74 W	1.484 38	1.473 36	1.279 17	1.242 03	1.096 30
75 Re	1.4410	1.429 97	1.236 03	1.2041	1.0587
76 Os	1.398 66	1.388 59	1.194 90	1.168 84	1.022 96
77 Ir	1.3598	1.348 47	1.155 40	1.132 97	0.988 76
78 Pt	1.321 55	1.310 33	1.117 58	1.099 74	0.955 99
79 Au	1.285 02	1.273 77	1.081 28	1.068 01	0.924 61
80 Hg	1.249 51	1.238 63	1.046 52	1.037 70	0.8946
81 Tl	1.216 26	1.204 93	1.012 99	1.008 22	0.865 71
82 Pb	1.184 08	1.172 58	0.980 83	0.980 83	0.838 01
83 Bi	1.153 01	1.141 50	0.950 02	0.953 24	0.811 43
90 Th	0.965 85	0.954 05	0.763 56	0.791 92	0.651 76
91 Pa	0.9427	0.9309	0.7407	0.7721	0.6325
92 U	0.920 62	0.908 74	0.718 51	0.753 07	0.613 59

(From *Smithsonian Physical Tables*.)

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