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Atomic data for the elements of the 5d-sequence

ABSTRACT

A review is given of the availability of atomic data for the elements of the 5d-sequence and of the reliability of these data.

AVAILABILITY OF DATA

Most of the data concerned were obtained in the thirties, and these investigations were limited to the lower stages of ionization, in which the ground configurations are $5d^{n-2}6s^2$ or $5d^{n-1}6s$. In these systems the lowest odd configurations are $5d^{n-2}6s6p$ and $5d^{n-1}6p$. For higher stages of ionization the $5d^n$ configuration ($0<n<10$) will be the lower one. These data were very carefully compiled by Charlotte E. Moore in the Circular of the National Bureau of Standards 467 (1958) but sometimes the data were of somewhat low quality. Initially in the 3d-sequence the situation was the same but in the sixties, seventies and early eighties very many spectra were (re)analysed. This revival was made possible by the introduction of large computer systems to calculate the complex structure of d^n-systems. The difference between the 3d- and 5d-elements, however, is that in 3d-systems the electrostatic interactions dominate the energy-level structure, while for 5d-systems the magnetic influence, which is more difficult to describe theoretically, is more important. This effect is due to the larger nuclear charge. For this reason there are considerably less data available for the 5d-elements than in the 3d-sequence. This is shown in tables I and II.

Those 5d-spectra that have been analysed thus far are the least complex. Only $5d^n$ configurations (starting to be the ground configuration from the III-spectra)with small n or n close to 10 were investigated. This is shown in table III.

RELIABILITY OF DATA

Reliability of data is difficult to prove without re-analysing or re-investigating the spectra. This, however, is seldom done. Sometimes there are suspicions about the correctness of an analysis on theoretical or other grounds. After calculations of the average energy of the d^9 and d^8s configurations by Edlén doubts were raised about the correctness of the published abalysis of Hg IV in which the ground term belongs to $5d^86s$, while in the calculations $5d^9$ definitely is the lowest one. A recent analysis by Joshi et al. (1989) shows that Edlén's doubts were justified. The earlier (faulty) and the new (completely revised) analysis of Hg IV are given in table IV.

After the analysis of Tl III and Pb IV by Gutmann and Crooker (1973) some revision was made by us in the spectrum of Bi V also (Raassen et al. 1989). The changes were, in this case, supported by the isoelectronic trend from Tl III to Bi V.

A new tool for proving the correctness will be parametric calculations along isoelectronic as well as isoionic sequences using the recently introduced complete sets of operators (Hansen et al. 1988a and 1988b) and (Uylings et al. 1989). Inclusion of the recently developed magnetic operators is essential for calculations in 5d-spectra. A simple example is given in table V. It shows the calculation of the d^9s configuration in the 3d- as well as in the 5d-sequence.

CONCLUSION

- Most of the spectra of higher stages of ionization and with more complex d^n ground configurations in the 5d-sequence are still unknown.
- Analyses done in the past need reinvestigation.
- Parametric treatment using a complete set of operators is helpful to find errors in former analyses and to analyse unknown spectra.

Table I Percentage of levels known in lowest even configurations.

	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As
I	>90	>75	>75	>75	>90	>90	100					
II	100	>90	>90	>90	100	>90	>90	100				
III	100	100	>90	>75	>90	100	100	100	100			
IV	100	100	100	>90	100	>90	100	100	>90	100		
V		100	100	100	100	100	>90	100	100	>90	100	
VI			100	100	100	100	100	>90	100	100	>90	100
VII				100	100	100	>90	100		100	100	100
VIII					>90	100	100					100

Table II Percentage of levels known in lowest even configurations.

	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi
I	>90	>90	>90	>90	>90	>90	100					
II	>90	>90	>90	>90	>75	>90	>90	100				
III	>90		>90*					>90	100			
IV	100	100	100						>90*	100		
V		100	100						>90*	>90*	100	
VI			100							>90*	>90*	100
VII				100							>90*	>90*
VIII					100							>90*

* = publication in preparation

Table III Number of configurations investigated.

	d^1	d^2	d^3	d^4	d^5	d^6	d^7	d^8	d^9	d^{10}
3d	5	6	6	5	5	4	4	6	5	4
5d	5	3	1	1				4	5	4

Table IV

Hg IV (old)

Config.	Desig.	J	Level
$5d^8(^3F)6s$	6s ^4F	4½	0
		3½	7557
		2½	12084
		1½	15438
$5d^9$	$5d^9$ ^2D	2½	2192
		1½	10376
$5d^7$ $6s^2$	$6s^2$ ^4F	4½	5653
		3½	7897
		2½	9476
		1½	10592
$5d^8(^3P)6s$	6s′ ^4P	2½	21011
		1½	23270
		0½	24564
$5d^7$ $6s^2$	$6s^2$ ^4P	2½	24054
		1½	25001
		0½	25802
		4½	42131
		2½,3½	44599
		3½	53342
		3½	55664
		2½	57122
		3½	57270
		3½	59490
$5d^8(^3F)6p$	6p $^4F^o$	4½	70567
		3½	75655
		2½	79688
		1½	82884
$5d^8(^3F)6p$	6p $^4G^o$	5½	74419
		4½	81039
		3½	87825
		2½	92237
		3½	74702
		3½	75388
		2½	75772
		3½	77045
		3½	78556
		3½	79919
$5d^8(^3F)6p$	6p $^4D^o$	3½	85056
		2½	88216
		1½	89513
		0½	90327
		2½	85091
		3½	86380
		1½,2½	87185
		2½	91752
		1½,2½	101826
		2½	102255
		2½	102353
		1½,2½	106210
		2½	106385
		1½	106748
		1½,2½	108798
		2½	113648
		2½	114508

Hg IV (new)

Config.	J	Level
$5d^9$	5/2	0
	3/2	15685
$5d^86s$	9/2	60137
	7/2	66108
	5/2	69941
	3/2	71761
	5/2	77674
	7/2	78852
	1/2	82389
	3/2	83914
	5/2	86029
	3/2	88899
	9/2	92352
	7/2	93179
	1/2	93405
	3/2	100153
	5/2	100911
	1/2	-
$5d^86p$	7/2	130813
	9/2	133616
	3/2	138710
	5/2	139262
	5/2	146768
	7/2	147286
	1/2	-
	11/2	150231
	3/2	152092
	9/2	152492
	7/2	153354
	5/2	154125
	1/2	154238
	5/2	155956
	3/2	156773
	7/2	159698
	5/2	160553
	9/2	161406
	1/2	162542
	7/2	164146
	3/2	165069
	5/2	165172
	9/2	165900
	7/2	167726
	3/2	168415
	5/2	169343
	3/2	172765
	5/2	173046
	7/2	173307
	1/2	173589
	3/2	173841
	1/2	177882
	5/2	178025
	3/2	178149
	11/2	178694
	5/2	179890
	3/2	180159
	7/2	183308
	9/2	184942
	3/2	186779
	5/2	188791
	7/2	188868
	1/2	191225
	1/2	-
	3/2	-

Table V Experimental and calculated values in a $3d^94s$ and $5d^96s$ conf.

	$3d^94s$ (Ge V)			$5d^96s$ (Pb V)				
J	Exp.	Calc.		Exp.	Calc.		Calc.	
3	234231	234234	-3	110768	110845	-77	110764	4
2	235971	235966	5	114705	114592	113	114713	-8
1	238767	238767	0	132711	132577	134	132698	13
2	241947	241948	-1	135997	136083	-86	136003	-6
E_{av}		237275			121351		121351	
C_{ds}		2127			3141		3141	
Zeta		1813			8693		8693	
A_{mso}		0			0		81	
A_{ss}		0			0		0	

REFERENCES

Gutmann, F. and Crooker A.M., 1973 - Extensions in the Spark Spectra of Tl III and Pb IV. In: Ca. J. Phys., 51, 1823-1830.

Hansen, J.E., Uylings, P.H.M. and Raassen, A.J.J., 1988a - Parametric fitting with orthogonal operators. In: Physica Scripta, 37, 664-672.

Hansen, J.E., Raassen, A.J.J., Uylings, P.H.M. and Lister, G.M.S., 1988b - Parametric fitting to d^N configurations using orthogonal operators. In: Nucl. Instr. Methods Phys. Res._ B31, 134-138.

Joshi, Y.N., Raassen, A.J.J. and Arcimowicz, B., 1989 - Fourth spectrum of mercury: Hg IV. In: J. Opt. Soc. Am. B6, 534-538.

Raassen, A.J.J., Van der Valk, A.A. and Joshi, Y.N., 1989 - Revised and extended analysis of Bi V. In: J. Phys. B: At. Mol. Opt. Phys., 22, 13-20.

Uylings, P.H.M., Van het Hof, G.J. and Raassen, A.J.J., 1989 - Orthogonal operators for d^Ns configurations: definition and interpretation. In: J. Phys. B: At. Mol. Opt. Phys., 22, L1-L4.

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