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The Fourth Spectrum of Mercury: Hg IV

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Abstract—*The triply ionized mercury (Hg IV) is an Au III like-spectrum with $5d^9(^2D_{5/2})$ as its ground state. The spectrum was recorded on a 3-m normal incidence vacuum spectrograph at the Antigonish laboratory (Canada) using a triggered spark light source in the 300-2080Å wavelength region. The excited configuration(s) $5d^86p$ in the odd parity system and $5d^86s$ in the even parity system have been studied earlier. New configurations have been extended in our theoretical calculations made by Cowan's relativistic Hartree-Fock code with superposition of configurations involving $5d^9$ + $5d^8(6s + 7s + 8s + 6d + 7d)$ + $5d^76s^2$ in the even parity system and $5d^8(6p + 7p + 8p)$ + $5d^8(5f + 6f + 7f)$ + $5d^76s6p$ + $5p^5(d^{10} + d^96s)$ in the odd parity configurations. At present, we are investigating $5d^87s$, $5d^88s$ along with $5d^87p$ with the aid of theoretical prediction and recorded experimental data. Known energy level values have been used to optimize the energy parameters of least squares fitted (LSF) parametric calculations to interpret the observed level structure.*

Keywords*: Wavelengths, Energy level, Transition probability.*

1. INTRODUCTION AND EXPERIMENT

Spectroscopy is the analysis of light spectra and the manner in which light interacts with the matter. The fundamental measurement achieved in spectroscopy is the "Spectrum"–a plot between the measured light intensity and some other property of light [1]. The radiation(s) emitted during an electronic transition between the energy levels from an excited atom (or ion) in the form of discrete wavelengths (spectral lines) are inversely proportional to the difference of energy between those energy levels.

The ground state electronic configuration of triply ionized mercury is $5d^9$ has Au III like spectrum with $^2D_{5/2}$ as its ground most level. The excited state configurations of interest are $5d^8(6p + 7p + 8p)$ + $5d^8(5f + 6f + 7f)$ + $5d^76s6p$ + $5p^5(d^{10} + d^96s)$ in the odd parity configurations and $5d^9$ + $5d^8(6s + 7s + 8s + 6d + 7d)$ + $5d^76s^2$ in the even parity system. Previously, a total of 61 energy levels belonging to $5d^9$, $5d^86s$ and $5d^86p$ configurations have been reported by Joshi *et al*. [2] and Van der Valk *et al*. [3] which is also listed on the NIST ASD [4].

The vacuum ultraviolet spectra of mercury were recorded on a 3-m normal incidence spectrograph in the 300-2080Å region at the St. Francis Xavier University, Antigonish (Canada) using triggered spark source. The spectrograph is equipped with a holographic concave grating with 2400 lines per mm ruling giving first order inverse dispersion of 1.385 Å per mm. The measured and calibrated wavelengths are estimated to have accuracy of ± 0.006Å. The further experimental details can be found elsewhere [5].

2. THEORETICAL ASPECT

In the present work we have performed configuration interaction (CI) calculations using the Cowan's code [6].

The initial scaling of the Slater parameters was kept at 100 % of the Hartree-Fock values for the average energy of the configurations (E_{av}) and the spin–orbit interaction (ζ_{nl}) integrals. The Radial wave integral (F^k), exchange integral (G^k) and configuration interaction integral (R^k) were scaled to 85% of HFR values. This scaling gives reasonably good predictions.

3. RESULTS AND DISCUSSION

As mentioned-above, the *ab-initio* calculations by means of R. D. Cowan's code [6] were employed to predict the energy level structure as well as the associated wavelength and transition probabilities along with the cancellation factor. The independent analysis was carried out from beginning and we found that all the levels reported in ref. [2-3] were satisfactory and we confirmed them here in this present work with improved level fitting in the least squares fitted (LSF) parametric calculations. In addition to that, 13 out of 16 new energy levels of $5d^87s$ configuration have been established for the first time. The remaining three energy levels of the above configuration ($5d^87s$) with designations $5d^87s$ ($^2S_{1/2}$), $5d^87s$ ($^2G_{7/2}$) and $5d^87s$ ($^2G_{9/2}$) could not be identified. All the observed levels belonging to odd and even parity configurations are given in Table-1 and Table-2 respectively along with their LS-percentage compositions. The standard deviation(s) for odd and even parity levels were found to be 244 cm^{-1} and 229 cm^{-1} respectively.

Table 1: Observed and least squares fitted levels of odd parity configurations of Hg IV in cm^{-1}.

J	E(obs)	E(LSF)	diff.	LS-composition.
1/2	149585.4	149606.0	-20.6	26% 5p6 5d8 6p (<2>3P)4D + 19% 5p6 5d8 6p (<2>3P)2P
	154239.7	154543.0	-303.3	60% 5p6 5d8 6p (<2>3P)4P + 30% 5p6 5d8 6p (<2>3P)4D
	162543.3	162474.0	69.3	36% 5p6 5d8 6p (<2>1D)2P + 25% 5p6 5d8 6p (<2>3P)2S
	173589.4	173145.0	444.4	56% 5p6 5d8 6p (<2>3F)4D + 30% 5p6 5d8 6p (<2>3P)2P
	177883.4	177922.0	-38.6	49% 5p6 5d8 6p (<2>3P)2S + 17% 5p6 5d8 6p (<2>3P)4P
	191226.8	191588.0	-361.2	38% 5p6 5d8 6p (<2>1D)2P + 34% 5p6 5d8 6p (<2>3P)2P
	-	197219.0	-	64% 5p6 5d8 6p (<0>1S)2P + 10% 5p6 5d8 6p (<2>1D)2P
3/2	138711.0	138766.0	-55.0	26% 5p6 5d8 6p (<2>1D)2D + 22% 5p6 5d8 6p (<2>3P)4P
	152092.8	152331.0	-238.2	28% 5p6 5d8 6p (<2>3P)4D + 20% 5p6 5d8 6p (<2>3F)4D
	156773.6	156335.0	438.6	21% 5p6 5d8 6p (<2>3P)4D + 16% 5p6 5d8 6p (<2>1D)2D
	165069.3	164577.0	492.3	35% 5p6 5d8 6p (<2>3P)2P + 26% 5p6 5d8 6p (<2>3F)4D
	168416.1	168451.0	-34.9	33% 5p6 5d8 6p (<2>1D)2P + 32% 5p6 5d8 6p (<2>3F)4F
	172766.1	172709.0	57.1	24% 5p6 5d8 6p (<2>3F)2D + 16% 5p6 5d8 6p (<2>3F)4D
	173841.9	173747.0	94.9	25% 5p6 5d8 6p (<2>3P)2D + 25% 5p6 5d8 6p (<2>3P)4S
	178150.2	178147.0	3.2	37% 5p6 5d8 6p (<2>3F)2D + 22% 5p6 5d8 6p (<2>3P)2P
	180160.5	180163.0	-2.5	41% 5p6 5d8 6p (<2>3P)4S + 31% 5p6 5d8 6p (<2>3P)2D
	186780.2	186374.0	406.2	23% 5p6 5d8 6p (<2>1D)2P + 21% 5p6 5d8 6p (<2>1D)2D
	-	213534.0	-	77% 5p6 5d8 6p (<0>1S)2P + 7% 5p6 5d8 6p (<2>3P)2D
5/2	139262.3	139259.0	3.3	28% 5p6 5d8 6p (<2>1D)2F + 17% 5p6 5d8 6p (<2>3P)4D
	146768.5	146675.0	93.5	44% 5p6 5d8 6p (<2>3F)4D + 33% 5p6 5d8 6p (<2>3F)4F
	154125.3	153931.0	194.3	27% 5p6 5d8 6p (<2>3P)4P + 27% 5p6 5d8 6p (<2>3F)4G
	155956.5	156116.0	-159.5	56% 5p6 5d8 6p (<2>3F)2D + 9% 5p6 5d8 6p (<2>3P)2D
	160554.1	160827.0	-272.9	26% 5p6 5d8 6p (<2>3P)2D + 22% 5p6 5d8 6p (<2>3F)2D
	165173.9	164945.0	228.9	26% 5p6 5d8 6p (<2>3F)4D + 20% 5p6 5d8 6p (<2>3F)4F
	169343.3	169446.0	-102.7	24% 5p6 5d8 6p (<2>3F)4G + 21% 5p6 5d8 6p (<2>1D)2D
	173047.6	173222.0	-174.4	36% 5p6 5d8 6p (<2>3F)2F + 16% 5p6 5d8 6p (<2>1D)2F
	178026.3	178025.0	1.3	45% 5p6 5d8 6p (<2>3P)4D + 31% 5p6 5d8 6p (<2>3P)2D
	179892.0	179594.0	298.0	69% 5p6 5d8 6p (<2>1G)2F + 6% 5p6 5d8 6p (<2>1D)2D
	188792.1	188870.0	-77.9	28% 5p6 5d8 6p (<2>1D)2D + 21% 5p6 5d8 6p (<2>3F)2F
7/2	130813.8	130723.0	90.8	61% 5p6 5d8 6p (<2>3F)4D + 18% 5p6 5d8 6p (<2>3F)4F
	147286.1	147465.0	-178.9	60% 5p6 5d8 6p (<2>3F)4G + 16% 5p6 5d8 6p (<2>3F)2G
	153353.9	153380.0	-26.1	56% 5p6 5d8 6p (<2>3F)2F + 21% 5p6 5d8 6p (<2>3F)4D
	159698.8	159873.0	-174.2	44% 5p6 5d8 6p (<2>1D)2F + 28% 5p6 5d8 6p (<2>3P)4D
	164147.4	163757.0	390.4	59% 5p6 5d8 6p (<2>1G)2F + 15% 5p6 5d8 6p (<2>3F)4F
	167726.6	167835.0	-108.4	45% 5p6 5d8 6p (<2>3F)4F + 23% 5p6 5d8 6p (<2>3F)2F
	173308.4	173489.0	-180.6	46% 5p6 5d8 6p (<2>3P)4D + 31% 5p6 5d8 6p (<2>3F)2G
7/2	183310.1	183202.0	108.1	72% 5p6 5d8 6p (<2>1G)2G + 20% 5p6 5d8 6p (<2>1G)2F
	188871.4	188976.0	-104.6	46% 5p6 5d8 6p (<2>1D)2F + 20% 5p6 5d8 6p (<2>3F)2G
9/2	133616.5	133473.0	143.5	39% 5p6 5d8 6p (<2>3F)2G + 32% 5p6 5d8 6p (<2>3F)4G
	152493.1	152411.0	82.1	66% 5p6 5d8 6p (<2>3F)4F + 27% 5p6 5d8 6p (<2>3F)2G
	161408.4	161750.0	-341.6	78% 5p6 5d8 6p (<2>1G)2H + 15% 5p6 5d8 6p (<2>1G)2G
	165901.7	166145.0	-243.3	64% 5p6 5d8 6p (<2>3F)4G + 29% 5p6 5d8 6p (<2>3F)2G
9/2	184944.3	184960.0	-15.7	79% 5p6 5d8 6p (<2>1G)2G + 14% 5p6 5d8 6p (<2>1G)2H
11/2	150230.7	150409.0	-178.3	94% 5p6 5d8 6p (<2>3F)4G + 6% 5p6 5d8 6p (<2>1G)2H
J	E(obs)	E(LSF)	diff.	LS-composition.
11/2	178696.5	178938.0	-241.5	93% 5p6 5d8 6p (<2>1G)2H + 6% 5p6 5d8 6p (<2>3F)4G

Table-2: Observed and least squares fitted levels of even parity configurations of Hg IV in cm^{-1}.

J	E(obs)	E(LSF)	diff.	LS-composition.
1/2	82390.9	82346.0	44.9	82% 5p6 5d8 6s (<2>3P)4P + 15% 5p6 5d8 6s (<0>1S)2S
	93406.0	93398.0	8.0	87% 5p6 5d8 6s (<2>3P)2P + 7% 5p6 5d8 6s (<2>3P)4P + 5% 5p6 5d8 6s (<0>1S)2S
	-	124598.0	-	79% 5p6 5d8 6s (<0>1S)2S + 11% 5p6 5d8 6s (<2>3P)4P + 9% 5p6 5d8 6s (<2>3P)2P
	261617.1	261581.0	36.1	61% 5p6 5d8 7s (<2>3P)4P + 15% 5p6 5d8 7s (<0>1S)2S + 12% 5p6 5d8 7s (<2>3P)2P + 4% 5p6 5d8 6d (<2>3P)4D
	267000.5	267077.0	-76.5	76% 5p6 5d8 7s (<2>3P)2P + 22% 5p6 5d8 7s (<2>3P)4P
	-	305310.0	-	78% 5p6 5d8 7s (<0>1S)2S + 11% 5p6 5d8 7s (<2>3P)4P + 6% 5p6 5d8 7s (<2>3P)2P
3/2	71763.1	71740.0	23.1	48% 5p6 5d8 6s (<2>1D)2D + 29% 5p6 5d8 6s (<2>3F)4F + 14% 5p6 5d8 6s (<2>3P)2P + 8% 5p6 5d8 6s (<2>3P)4P
	83915.7	83874.0	41.7	62% 5p6 5d8 6s (<2>3P)4P + 30% 5p6 5d8 6s (<2>3F)4F + 7% 5p6 5d8 6s (<2>3P)2P
	88899.7	88984.0	-84.3	47% 5p6 5d8 6s (<2>3P)2P + 29% 5p6 5d8 6s (<2>3P)4P + 20% 5p6 5d8 6s (<2>3F)4F
	100155.3	100094.0	61.3	48% 5p6 5d8 6s (<2>1D)2D + 29% 5p6 5d8 6s (<2>3P)2P + 21% 5p6 5d8 6s (<2>3F)4F
	246421.2	246102.0	319.2	39% 5p6 5d8 7s (<2>1D)2D + 20% 5p6 5d8 7s (<2>3F)4F + 16% 5p6 5d8 7s (<2>3P)2P + 9% 5p6 5d8 6d (<2>3F)4D
	260784.8	260565.0	219.8	44% 5p6 5d8 7s (<2>3F)4F + 37% 5p6 5d8 7s (<2>3P)2P + 14% 5p6 5d8 7s (<2>3P)4P
	266217.0	266240.0	-23.0	58% 5p6 5d8 7s (<2>3P)4P + 17% 5p6 5d8 7s (<2>3P)2P + 8% 5p6 5d8 6d (<2>3P)2P + 4% 5p6 5d8 6d (<2>3P)2D
	275089.3	275462.0	-372.7	50% 5p6 5d8 7s (<2>1D)2D + 28% 5p6 5d8 7s (<2>3F)4F + 19% 5p6 5d8 7s (<2>3P)2P
5/2	69942.4	70017.0	-74.6	44% 5p6 5d8 6s (<2>3P)4P + 39% 5p6 5d8 6s (<2>1D)2D + 15% 5p6 5d8 6s (<2>3F)4F
	77675.2	77627.0	48.2	73% 5p6 5d8 6s (<2>3F)4F + 14% 5p6 5d8 6s (<2>3P)4P + 13% 5p6 5d8 6s (<2>3F)2F
	86031.1	86039.0	-7.9	46% 5p6 5d8 6s (<2>3F)2F + 34% 5p6 5d8 6s (<2>3P)4P + 19% 5p6 5d8 6s (<2>1D)2D

	100912.6	100980.0	-67.4	41% 5p6 5d8 6s (<2>1D)2D + 39% 5p6 5d8 6s (<2>3F)2F
				+ 12% 5p6 5d8 6s (<2>3F)4F + 8% 5p6 5d8 6s (<2>3P)4P
	245714.9	245946.0	-231.1	47% 5p6 5d8 7s (<2>1D)2D + 29% 5p6 5d8 7s (<2>3P)4P
				+ 13% 5p6 5d8 7s (<2>3F)4F + 8% 5p6 5d8 7s (<2>3F)2F
	251492.9	251728.0	-235.1	57% 5p6 5d8 7s (<2>3F)4F + 41% 5p6 5d8 7s (<2>3F)2F
	260323.9	260356.0	-32.1	50% 5p6 5d8 7s (<2>3P)4P + 30% 5p6 5d8 7s (<2>3F)2F
				+ 15% 5p6 5d8 7s (<2>3F)4F
	275795.3	275478.0	317.3	49% 5p6 5d8 7s (<2>1D)2D + 19% 5p6 5d8 7s (<2>3F)2F
				+ 18% 5p6 5d8 7s (<2>3P)4P + 13% 5p6 5d8 7s (<2>3F)4F
7/2	66109.0	65923.0	186.0	57% 5p6 5d8 6s (<2>3F)4F + 37% 5p6 5d8 6s (<2>3F)2F
				+ 6% 5p6 5d8 6s (<2>1G)2G
	78853.5	78877.0	-23.5	55% 5p6 5d8 6s (<2>3F)2F + 43% 5p6 5d8 6s (<2>3F)4F
	93182.5	93036.0	146.5	91% 5p6 5d8 6s (<2>1G)2G + 8% 5p6 5d8 6s (<2>3F)2F
	236701.5	236955.0	-253.5	66% 5p6 5d8 7s (<2>3F)2F + 28% 5p6 5d8 7s (<2>3F)4F
				+ 5% 5p6 5d8 7s (<2>1G)2G
	251646.1	251439.0	207.1	70% 5p6 5d8 7s (<2>3F)4F + 29% 5p6 5d8 7s (<2>3F)2F
	-	269688.0	-	92% 5p6 5d8 7s (<2>1G)2G
9/2	60137.8	60291.0	-153.2	96% 5p6 5d8 6s (<2>3F)4F + 4% 5p6 5d8 6s (<2>1G)2G
	92355.0	92503.0	-148.0	95% 5p6 5d8 6s (<2>1G)2G + 4% 5p6 5d8 6s (<2>3F)4F
J	E(obs)	E(LSF)	diff.	LS-composition.
9/2	235937.0	235735.0	202.0	91% 5p6 5d8 7s (<2>3F)4F + 4% 5p6 5d8 7s (<2>1G)2G
	-	269644.0	-	93% 5p6 5d8 7s (<2>1G)2G + 4% 5p6 5d8 7s (<2>3F)4F

4. CONCLUSION

A comprehensive interpretation of the spectrum of triply ionized mercury (Hg IV) has been carried out. The analysis is well supported by theoretical predictions and experimental data in the wavelength region 300Å to 2080Å. The earlier reported levels of even and odd parity configurations have been confirmed and 13 new levels based on the identification of 62 transitions have been established. Only three levels of the newly studied configuration $5d^8 7s$ could not be established.

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REFERENCES

[1] Brian, C. Smith., "Quantitative Spectroscopy: Theory Practice", *Academic Press*, California, USA, (2002).

[2] Joshi, Y. N., Raassen, A. J. J., and Arcimowicz B., "Fourth Spectrum of Mercury: Hg IV", *J. Opt. Soc. Am. B* 6, 534–538 (1989).

[3] Van der Valk, A. A., Raassen, A. J. J., and Joshi, Y. N., "Analysis of the $5d^8 6s$ and $5d^8 6p$ Configurations in Hg IV", *J. Opt. Soc. Am. B* **7**, 1182–1189 (1990).

[4] Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2017). *NIST Atomic Spectra Database (ver. 5.5.1)*, National Institute of Standards and Technology, Gaithersburg, MD, USA.

[5] Raassen, A. J. J., Joshi, Y. N., Tauheed, A., "Analysis of the $5d^8$ and $5d^7 6p$ configurations of the fifth spectrum of mercury: Hg V" - *Physica Scripta,* 1991.

[6] Cowan, R. D., "The theory of atomic structure and spectra", University of California Press, Berkeley (1981) and Cowan code package for Windows by Kramida, A., available from *http://das101.isan.troitsl.ru/COWAN*