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Analysis of the $(5d^8 + 5d^76s)$–$5d^76p$ Transition Array of Triply-Ionized Gold (Au IV)

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Abstract

The sliding and triggered spark spectrum of gold has been observed in the wavelength range of 554–2080 Å, where 657 lines have been classified as $5d^76s$–$5d^76p$ transitions. Twenty-nine of the 34 levels of the $5d^76s$ configuration have been found and the known levels of $5d^76p$ are increased from 64–95. In both parities, noticeable perturbations are due to configuration mixings within the groups $(5d + 6s)^8$ and $(5d + 6s)^76p$. Theoretical oscillator strengths are given for a selected number of strong Au IV lines.

1. Introduction

The first analysis of the spectrum of triply ionized gold led to the classification of 196 lines as transitions between 64 levels of $5d^76p$ and the 8 lowest levels of the ground configuration $5d^8$ [1]. This, and similar works in the Os I isoelectronic sequence (Hg V [2], Tl VI [3], Pb VII and Bi VIII [4]), was derived from triggered spark spectra photographed on normal incidence spectrographs at Antigonish and Amsterdam. Later, the complex spectral region where $6s$–$6p$, $6p$–$7s$ and $6p$–$6d$ transitions of different ion stages overlap was investigated. The case of Hg V [5] was considered first and the advances in Au IV, Tl VI and Pb VII led to helpful extrapolations for unraveling Pt III [6]. In the meantime, the importance of configuration mixings in $(5d + 6s)^N$ groups of moderately charged ions was evaluated. In the Ir I sequence, different mixing effects on the $^2D_{5/2}$ and $^2D_{3/2}$ levels of $5d^9$ was first displayed in [7] and, in the osmium sequence, the relative importance of effective parameters and Slater integrals ($R^2(5d^2,5d6s)$ in least squares fits of $5d^76s$ was recently analyzed [8]. A preliminary theoretical survey of $(5d + 6s)^8$ by means of orthogonal operators and generalized least squares techniques collected all low even levels known in 1992 and displayed empirical regularities in the Os I sequence [9].

The present publication extends the description of Au IV from 196–700 classified lines and improves the earlier interpretation of the odd parity levels, the rms deviation being reduced from 263–185 cm^{-1}, by including explicitly $5d^66s6p$ and $5d^56s^26p$ in the vector basis set.

2. Experimental data

The analysis of Au IV presented in this paper is primarily based on the accurate wavelength list obtained from the gold spectrum photographed in the 1020–1930 Å region on a 10.7 m normal incidence spectrograph at the NBS laboratory almost 15 years ago. The plate factor of the spectrograph was 0.78 Å/mm and the source used was a sliding spark. The spark was operated under various conditions. In absence of known lines of Au IV in the observed range, the intensity behaviour of classified lines of Au I, Au II and Au III helped in selecting the probable $5d^76s$–$5d^76p$ transitions of Au IV. The semi-automatic comparator at Observatoire de Paris–Meudon was used for measuring the line positions. Reference wavelengths were provided by a copper hollow cathode spectrum recorded on the same plates and also by internal standards of impurity elements (Si, C, N and Al). Second order polynomials led to wavelengths uncertainties of 0.007 Å. Recently, a comparison with wavelengths measured (or calculated by Ritz principle) at Lund university by means of hollow cathode emission and Fourier transform spectrometry confirmed the photographic measurements for Au I and Au II lines present on the plates. Only 6 out of 47 Au I and Au II lines show wavelength disagreements larger than 0.007 Å. The NBS spectrum data were supplemented by additional gold plates taken on a 3 m normal incidence spectrograph at the Antigonish laboratory in the 554–2080 Å region. The source used was a triggered spark and the experimental details appeared in an earlier paper [1]. The spectrum is very rich in lines and there are many cases of blends and perturbations by close lines.

3. Analysis

Isoionic and isoelectronic regularities in the energy differences between lowest levels of $5d^N6s^M$ configurations were used to predict the interval $5d^76s\,^5F_5$–$5d^8\,^3F_4$ at 51 300 cm^{-1} with a 5‰ accuracy [9]. Line strengths for the array $5d^76s$–$5d^76p$ were calculated and it was found that neglecting the mixing effects with close configurations in both parities, viz. $5d^8 + 5d^66s^2$ and $5d^66s6p + 5d^76s^26p$, did not seriously effect a qualitative agreement between the line strengths and the observed intensities. In the final step of the analysis, the conventional parametric description, which used the same energy matrices as in [10–12], was replaced by selected orthogonal operators for electrostatic and magnetic interactions, as described in [8, 9]. The improved accuracy was useful when searching for those upper levels of $5d^76s$ which have few transitions. Unfortunately, the analysis could not be pursued to its very end. Most of the levels built on the high parent term 1^2D of $5d^7$ are still missing and therefore, $5d^8\,^1S_0$ could not be identified either. The 37 known even levels are given in Table III.

In the odd parity all levels of $5d^76p$ reported in [1], except two, have been confirmed and 34 new levels have been found. In searching for the $J = 2$ level predicted at $E_{calc} = 160\,010\,\mathrm{cm}^{-1}$ in [1], we could not find any new level at an acceptable energy. We have now found that the 160042 level (given as $J = 3$ in [1]) decays to 4 levels with $J = 1$ (including an expected line to $5d^8\,^3P_1$) and to 3 levels with $J = 4$ and the double attribution $J = 2$ and $J = 3$ is well-established. Both levels have different wavefunctions and their transitions with the same low even level have different line strengths. An indication of a double classification is given in Table I, only when both line strengths have the same order of magnitude. The two $J = 2$ and $J = 3$ levels are so close that we could not derive different energy values from the classified lines. Another case of near-degeneracy had been already found in the same configuration, as one $J = 1$ and one $J = 3$ levels appeared at the same energy, $164\,234.4\,\mathrm{cm}^{-1}$ [1]. The $6s$–$6p$ transitions helped in deriving two different level values at 164234.15 ($J = 1$) and 164233.10 ($J = 3$). Their transitions to the $J = 2$ level at $78\,137\,\mathrm{cm}^{-1}$ have similar line strengths and, indeed, the corresponding line at 1161.485 Å is broader than others. All $J = 6$ levels of the $5d^76p$ configuration have been found from few, but strong, transitions, but their are still problems with the $J = 7$ level. There is none unclassified line having a typical Au IV character near 1190 Å, where the transition $5d^76p\,^3I_7$–$5d^76s\,^3H_6$ is predicted to appear. Isoelectronic regularities for $^3I_7$ are in favour of a double classification for the line at 1190.889 Å, already classified as 67853 (4)–151824 (5). This is the strongest Au IV line within a 20 Å range around 1190 Å (i.e. an energy range which is 4 times larger than the rms error of the theoretical predictions of energy levels).

There are 657 lines reported in Table I.A, for which 677 transitions are given. However, double classifications has only been given to lines where both components are predicted to contribute to the observed intensity. The intensities, in arbitrary units, were determined in the densitometer processing of 4 different plates. They are not consistent throughout Table I.A and had to be completed by visual estimates in some parts. Comparing them is only meaningful in a restricted wavelength range. A '*' indicates lines, for which the measured wavelengths and the wavelengths derived from the energy levels differ more than 0.010 Å. When fitting the level values, all wavenumbers have been given equal weights in the 1930–1080 Å range and the deviations $\Delta\lambda$ are larger at longer wavelengths. The average uncertainties are 0.25 and $0.40\,\mathrm{cm}^{-1}$ for the even and odd levels, respectively and the estimated maximum uncertainty is $0.70\,\mathrm{cm}^{-1}$. Oscillator strengths have been calculated by means of Cowan's atomic codes [14] and the 23 lines with $gf > 2$ are listed in Table II, together with the 4 strongest lines in the range 1930–1600 Å.

4. Theoretical interpretation

Even if the energy ranges of $5d^8$ and $5d^76p$ overlap slightly, the gap between the highest levels of $5d^8$ and the lowest levels of $5d^76s$ is larger than $28\,000\,\mathrm{cm}^{-1}$ for any individual J-values. Various parametric fittings of $5d^76s$ have been performed from Os I to Pb VII in order to compare the ("far" and "close") configuration (or "weak" and "strong") mixing effects. It was concluded in [8] that Au IV is the spectrum where the effective parameters T_{dds} and A_{MSO} improve the rms error on the $5d^76s$ levels as much as the Slater parameter $R^2(5d^2,6s^2)$ and $R^2(5d^2,5d6s)$ do in the full treatment of $5d^8 + 5d^76s + 5d^66s^2$. The small standard errors in the fitted $R^2(5d^2,5d6s)$ $(-24044 \pm 749\,\mathrm{cm}^{-1})$ and A_{MSO} $(58.7 \pm 3\,\mathrm{cm}^{-1})$ support the treatment of "weak" and "strong" interactions together in the present case. In Table III, the experimental levels of $5d^8$ and $5d^76s$ are compared with theoretical values. Forty-three parameters, 25 of them being fixed or constrained according to the results of [8], lead to deviations reported in the third column of the Table. The leading components in *LS*-coupling and the percentages of components pertaining to the three low even configurations complete the Table. Among the known levels, the largest mixings are noticed for $5d^76s\,^3P_0$ (3.3%).

In odd configurations, only the conventional approach of configuration interaction is still possible to apply, and the mixing of $5d^N6p$, $5d^{N-1}6s6p$ and $5d^{N-2}6s^26p$ has been studied so far in very few cases [13]. In Au IV, the large value of $R^2(5d^2,5d6s)$ fitted in the even parity configurations and the *ab initio* values of the Slater integrals $R^2(5d6p,6s6p)$ and $R^1(5d6p,6p6s)$ derived from the HXR method [14] claim for extending the vector basis from the 110 levels of $5d^76p$ to the 684 levels of the group $(5d + 6s)^76p$. By keeping the average energies of the configurations $5d^66s6p$ and $5d^56s^26p$ fixed so that their lowest levels appear near 185000 and $270\,000\,\mathrm{cm}^{-1}$, respectively, 40 parameters (Table IV) have been fitted from 94 energy levels (Table V). The parameters of both these unknown configurations were constrained in such a way that, for any Slater integral, the scaling factor (ratio of fitted/*ab initio* values) is the same as for $5d^76p$. All seven Slater parameters taking into account the close configuration mixing have been reduced to one, the same scaling being assumed for all. This leads to a value $R^2(5d^2,5d6s) = -24\,546 \pm 1043\,\mathrm{cm}^{-1}$, in very good agreement with the opposite parity results. The improvement of the rms deviation from 263–$185\,\mathrm{cm}^{-1}$ is not large enough for withdrawing the conclusions of [1] on the importance of effective magnetic parameters in $5d^76p$. The present analysis only implies that $(5d + 6s)^N6p$ should be the right basis for developing new sets of effective operators in odd parity levels of moderately charged ions.

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Table I.A. *Classified lines of Au IV in the* $5d^76s$–$5d^76p$ *transition array*

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1916.383	52181.63	40	*	79506	2	131688	3	
1914.106	52243.72	30		78137	2	130380	1	
1911.074	52326.59	40	*	97092	5	149418	6	
1909.700	52364.26	50		67853	4	120217	4	
1894.153	52794.04	20	*	79506	2	132300	2	
1893.326	52817.11	30	•	89582	2	142398	3	
1891.925	52856.23	20	*	79444	1	132300	2	
1875.221	53327.05	10	•	78361	4	131688	3	
1855.547	53892.45	40	*	79506	2	133398	3	1
1846.258	54163.61	30		78137	2	132300	2	
1834.476	54511.49	25		85798	4	140309	4	
1830.087	54642.22	70		67853	4	122495	5	
1811.531	55201.93	30		85107	5	140309	4	
1809.560	55262.06	50	•	78137	2	133398	3	
1800.224	55548.64	10		89582	2	145130	1	
1796.011	55678.94	1		78361	4	134040	4	
1790.645	55845.80	1	•	102513	2	158358	3	
1789.917	55868.51	60		75819	3	131688	3	2
1782.102	56113.49	20	•	83574	0	139687	1	
1772.824	56407.18	1		95882	4	152289	3	
1771.408	56452.27	30		63765	3	120217	4	
1770.509	56480.94	40		75819	3	132300	2	
1768.911	56531.97	10	*	100468	4	157000	3	
1766.754	56600.97	5		85798	4	142398	3	
1760.225	56810.91	10	•	102513	2	159323	1	
1741.815	57411.36	72		72968	1	130380	1	
1736.682	57581.07	76	•	75819	4	133398	3	
1735.000	57636.90	66	•	85798	4	143434	5	
1732.531	57719.03	58	•	92583	2	150301	3	
1727.791	57877.37	72	•	79506	2	137383	2	
1727.407	57890.24	58	*	100468	4	158358	3	
1725.657	57948.95	69		72968	1	130918	2	
1724.357	57992.63	1	*	95102	1	153094	2	
1717.612	58220.36	78		75819	3	134040	4	
1714.468	58327.14	5		85107	5	143434	5	
1712.347	58399.39	44	•	92583	2	150981	3	
1711.693	58421.68	33		83977	3	142398	3	
1702.097	58751.06	1	*	102513	2	161263	1	
1697.170	58921.62	50		85798	4	144719	3	
1696.452	58946.57	72		75093	5	134040	4	
1696.369	58949.44	66	*	92638	3	151587	2	
1694.761	59005.36	45		92583	2	151587	2	
1687.851	59246.92	1		78137	2	137383	2	
1685.450	59331.35	65		72968	1	132300	2	
1676.433	59650.47	67	*	92638	3	152289	3	

Table I.A. (*continued*)

λ (Å)	σ (cm⁻¹)	Int		E_{even}	J_e	E_{odd}	J_0	Note
1675.034	59700.27	19		92583	2	152282	1	
1674.868	59706.21	55		92583	2	152289	3	
1674.557	59717.30	1		92638	3	152356	4	
1674.151	59731.75	49		102513	2	162244	2	
1674.032	59736.00	35		79506	2	139242	2	
1672.297	59797.98	58		79444	1	139242	2	
1666.826	59994.28	62		103293	3	163287	4	
1664.974	60061.02	1	*	100468	4	160529	4	
1661.654	60181.02	37		79506	2	139687	1	
1661.571	60184.01	10		78361	4	138545	5	
1661.491	60186.91	43		95102	1	155289	2	
1658.013	60313.15	50		100468	4	160781	5	
1649.847	60611.67	49		89207	3	149818	4	
1648.963	60644.18	45		89582	2	150226	2	
1648.365	60666.17	57		91623	2	152289	3	
1646.915	60719.59	10		89582	2	150301	3	
1645.532	60770.63	32		100469	4	161239	3	
1640.521	60956.24	20		97092	5	158048	4	
1638.874	61017.51	77	*	89207	3	150226	2	+III
1636.799	61094.84	41		89207	3	150301	3	
1636.504	61105.87	73		78137	2	139242	2	
1633.794	61207.21	55		102939	1	164147	2	
1628.676	61399.57	1		89582	2	150981	3	
1624.666	61551.11	75		78137	2	139687	1	
1624.559	61555.15	62	*	83574	0	145130	1	
1624.320	61564.22	74	*	75819	3	137383	2	+I
1622.471	61634.39	52	*	102513	2	164146	2	
1618.513	61785.10	10	*	89803	1	151587	2	
1614.260	61947.89	47		78361	4	140309	4	
1613.581	61973.95	74		58243	4	120217	4	
1612.755	62005.70	33		89582	2	151587	2	
1612.210	62026.65	55		68891	3	130918	2	
1612.116	62030.28	60		81404	6	143434	5	
1611.870	62039.73	36		92638	3	154678	3	
1611.665	62047.62	20		95102	1	157149	2	
1610.395	62096.57	67	*	92583	2	154678	3	+III
1609.373	62136.00	30		83977	3	146113	4	
1600.496	62480.63	76	*	89803	1	152283	1	+III
1597.663	62591.41	20		92583	2	155174	1	
1596.159	62650.40	35		92638	3	155289	2	
1595.559	62673.97	24		97092	5	159766	6	
1594.875	62700.84	24		89582	2	152282	1	
1594.736	62706.32	25		92583	2	155289	2	
1592.438	62796.78	74		68891	3	131688	3	
1591.878	62818.89	23		100468	4	163287	4	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1590.027	62892.03	68		79506	2	142398	3	
1585.914	63055.13	25		91623	2	154678	3	
1585.234	63082.17	15		89207	3	152289	3	
1585.018	63090.77	30		67289	2	130380	1	
1583.541	63149.62	10		89207	3	152356	4	
1581.997	63211.27	18		102939	1	166151	2	
1580.005	63290.95	23		89803	1	153094	2	
1579.711	63302.73	37		103293	3	166596	4	d
1577.065	63408.93	73		68891	3	132300	2	
1576.719	63422.85	1		75819	3	139242	2	
1576.362	63437.19	39		97092	5	160529	4	
1576.004	63451.62	26		75093	5	138545	5	
1574.504	63512.07	30		89582	2	153094	2	
1571.623	63628.48	62		67289	2	130918	2	
1571.382	63638.27	5		102513	2	166151	2	
1570.693	63666.16	30		91623	2	155289	2	
1570.119	63689.46	48		97092	5	169781	5	
1568.734	63745.67	15		95102	1	158847	2	
1568.273	63764.40	20		100468	4	164233	3	
1566.553	63834.44	73		67853	4	131688	3	
1565.254	63887.38	30		89207	3	153094	2	
1563.532	63957.75	25		75093	5	139051	6	
1562.016	64019.84	78	*	85798	4	149818	4	+II
1561.594	64037.13	32		78361	4	142398	3	
1557.122	64221.02	28		95102	1	159323	1	
1556.368	64252.17	79	*	58243	4	122495	5	
1556.143	64261.47	70	*	66119	1	130380	1	
				78137	2	142398	3	
1554.946	64310.90	79		85107	5	149418	6	
1553.724	64361.50	22		92638	3	150700	3	
1552.833	64398.44	77		67289	2	131688	3	
1552.391	64416.75	20		92583	2	157000	3	d
1550.642	64489.44	10		75819	3	140309	3	
1550.278	64504.58	16	*	68891	3	133398	3	d
1548.054	64597.21	23		85798	4	150395	5	
1545.334	64710.93	30		85107	5	149818	4	
1543.248	64798.40	71		66119	1	130918	2	
1542.999	64808.84	10		102513	2	167322	1	
1540.843	64899.53	71		95882	4	160781	5	
1540.095	64931.07	27		85798	4	150728	4	
1538.195	65011.26	73		67289	2	132300	2	
1536.725	65073.44	75	*	78361	4	143434	5	
1536.187	65096.23	1		89582	2	154678	3	
1534.947	65148.85	69		68891	3	134040	4	
1534.125	65183.75	50		85798	4	150981	3	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1533.694	65202.08	20		103293	3	168495	3	
1533.398	65214.65	79	*	75093	5	140309	4	3
			*	79506	2	144719	3	
1531.684	65287.63	30		85107	5	150395	5	
1530.056	65357.07	15		95882	4	161239	3	
1529.726	65371.20	20	*	89803	1	155174	1	
1529.577	65377.56	38	*	91623	2	157000	3	?
1527.391	65471.13	15		89207	3	154678	3	
1527.050	65485.74	39		89803	1	155289	2	d
1525.665	65545.19	71		67853	4	133398	3	
1524.591	65591.38	20	*	89582	2	155174	1	
1523.843	65623.58	24		79506	2	145130	1	
1522.390	65686.20	61		79444	1	145130	1	
1521.910	65706.91	15		89582	2	155289	2	
1521.562	65721.92	75		64658	2	130380	1	
1520.336	65774.95	20		92583	2	158358	3	
1518.795	65841.66	74	*	83977	3	149818	4	
1514.545	66026.44	15		85798	4	151824	5	
1513.604	66067.50	25		103293	3	169360	4	
1512.647	66109.30	76		67289	2	133398	3	
1512.233	66127.40	25		100468	4	166596	4	
1512.108	66132.83	36		97092	5	163225	5	
1511.451	66161.59	25		95102	1	161263	1	
1511.013	66180.78	78		66119	1	132300	2	
1510.888	66186.25	80		67853	4	134040	4	
1510.682	66195.27	32		97092	5	163287	4	
1510.366	66209.12	22	*	102939	1	169149	1	
				92638	3	158847	2	S
1509.222	66259.31	79		64658	2	130918	2	
1509.110	66264.24	15		92583	2	158847	2	
1508.891	66273.83	73		72968	1	139242	2	
1507.740	66324.43	1		83977	3	150301	3	
1503.952	66491.49	25		85798	4	152289	3	d
1502.441	66558.35	76		85798	4	152356	4	+III
1501.972	66579.12	73		75819	3	142398	3	
1501.896	66582.51	B1		78137	2	144719	3	
1500.670	66636.91	3		102513	2	169149	1	
1498.827	66718.86	72		72968	1	139687	1	S
			*	85107	5	151824	5	
1498.086	66751.86	20		83977	3	150728	4	
1492.443	67004.23	1		83977	3	150981	3	
[1489.38]	[67142.0]	Bl		95102	1	162244	2	+III
1489.152	67152.34	65		63765	3	130918	2	
1487.556	67224.34	15		91623	2	158847	2	
1484.933	67343.11	60		95882	4	163225	5	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1484.862	67346.33	25		89803	1	157149	2	
1483.596	67403.80	30		92638	3	160042	2,3	
1483.566	67405.14	35		95882	4	163287	4	
1482.376	67459.28	50		92583	2	160042	2,3	S
1480.010	67567.12	50		89582	2	157149	2	
1479.292	67599.91	29		89582	2	157182	1	
1479.055	67610.72	34		83977	3	151587	2	
1478.378	67641.70	10		64658	2	132300	2	
1477.101	67700.17	40		91623	2	159323	1	
1475.976	67751.80	80		78361	4	146113	4	
1475.749	67762.20	75		103293	3	171055	3	d
1475.072	67793.28	70		89207	3	157000	3	
1473.922	67846.18	30		102513	2	170359	2	
1472.949	67891.04	35		92638	3	160529	4	
1472.272	67922.24	30		63765	3	131688	3	
1472.119	67929.31	30		100468	4	168397	5	
1471.830	67942.65	55		89207	3	157149	2	
1470.291	68013.74	85		81404	6	149418	6	
1470.016	68026.45	75		100468	4	168495	3	
1463.876	68311.82	75		83977	3	152289	3	
1463.256	68340.76	85		75093	5	143434	5	
1463.043	68350.69	25		95882	4	164233	3	
1462.444	68378.67	60		83977	3	152356	4	
1461.580	68419.11	75		91623	2	160042	3,2	
1460.017	68492.34	87		68891	3	137383	2	
1459.117	68534.59	85		63765	3	132300	2	
1455.434	68708.02	50		83574	0	152282	1	
1454.759	68739.91	65		64658	2	133398	3	
1454.000	68775.81	20		89582	2	158358	3	
1452.610	68841.62	85		89207	3	158048	4	
1451.551	68891.84	50		100468	4	169360	4	
1450.392	68899.38	20		75819	3	144719	3	
1450.953	68920.23	90		51297	5	120217	4	
1449.470	68990.73	85		81404	6	150395	5	
1446.822	69117.02	30		83977	3	153094	2	
1446.108	69151.11	85		89207	3	158358	3	
1443.728	69265.12	15		89582	2	158847	2	
1438.774	69503.60	82		97092	5	166596	4	
1438.439	69519.81	60		89803	1	159323	1	
1437.212	69579.14	70	*	103293	3	172873	4	
1436.440	69616.56	38		91623	2	161239	3	w
1436.097	69633.16	88		63765	3	133398	3	+III
1435.945	69640.56	60		91623	2	161263	1	
				89207	3	158847	2	
1435.515	69661.42	85		92583	2	162244	2	

Table I.A. *(continued)*

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1431.590	69852.39	70		103293	3	173146	2	
1426.651	70094.24	83		67289	2	137383	2	
1424.385	70205.72	60	*	102939	1	173146	2	
1423.928	70228.30	65		103293	3	173522	3	
1423.713	70238.90	10		89803	1	160042	2	
1422.994	70274.34	86		63765	3	134040	4	
1422.611	70293.31	75		75819	3	146113	3	
1421.443	70351.04	75		68891	3	139242	2	
1420.055	70419.79	84		81404	6	151824	5	
1419.252	70459.67	75		89582	2	160042	2	
1416.691	70587.03	75		100468	4	171055	3	
1416.006	70621.19	5		91623	2	162244	2	
1415.492	70646.80	Bl		92638	3	163287	4	+III
1414.591	70691.80	86		67853	4	138545	5	
1414.402	70701.26	82		83977	3	154678	3	
1414.161	70713.33	Bl		95882	4	166596	4	
1414.037	70719.52	60		79506	2	150226	2	S
1412.797	70781.59	15		79444	1	150226	2	
1412.533	70794.78	83		79506	2	150301	3	
1411.726	70835.28	55		89207	3	160042	3	
1409.484	70947.94	87		100468	4	171417	5	+III
1408.271	71009.07	84		102513	2	173522	3	
1408.067	71019.36	86		75093	5	146113	4	
1404.525	71198.44	91		51297	5	122495	5	
				85797	4	157000	3	
1403.583	71246.25	75		102513	2	173759	1	
1402.410	71305.81	60		97092	5	168397	5	
1402.102	71321.49	75	•	89207	3	160529	4	
1400.209	71417.90	83		68891	3	140309	4	
1399.442	71457.06	83		78361	4	149818	4	
1399.353	71461.59	55	•	89803	1	161263	1	
1398.437	71508.40	50		92638	3	164146	2	
1397.349	71564.09	50		92583	2	164146	2	
1396.761	71594.22	70		92638	3	164233	3	
1395.671	71650.12	65		92583	2	164233	3	
1395.536	71657.04	70		89582	2	161239	3	
1395.063	71681.37	65		89582	2	161263	1	
1389.794	71953.09	85		67289	2	139242	2	
1388.253	72032.99	35		89207	3	161239	3	
1387.329	72080.96	84		79506	2	151587	2	
1387.166	72089.42	85		78137	2	150226	2	
1386.132	72143.23	76		79444	1	151587	2	
1385.775	72161.80	Bl		72968	1	145130	1	+III
1384.636	72221.16	75	•	95102	1	167322	1	d
1383.731	72268.41	75		97092	5	169360	4	

Table I.A. *(continued)*

λ (Å)	σ (cm⁻¹)	Int		E_{even}	J_e	E_{odd}	J_0	Note
1381.835	72367.53	75		78361	4	150728	4	
1381.242	72398.59	83		67289	2	139687	1	
1381.146	72403.66	70	•	100468	4	172873	4	
1380.806	72421.47	70		97092	5	169513	6	
1380.432	72441.09	83		89803	1	162244	2	?
1380.159	72455.44	85		67853	4	140309	4	
1379.014	72515.57	85		95882	4	168397	5	?
1378.790	72527.37	75		102939	1	175467	1	
1378.167	72560.13	85		85798	4	158358	3	+III
1377.169	72612.76	75		95882	4	168495	3	
1377.031	72620.03	75		78361	4	150981	3	
1375.035	72725.41	75		64658	2	137383	2	
1374.078	72776.09	75		79506	2	152282	1	
1372.904	72838.32	80		79444	1	152282	1	
1372.789	72844.44	83		78137	2	150981	3	
1370.979	72940.56	55		85107	5	158048	4	
1369.435	73022.82	50		83977	3	157000	3	
1369.172	73036.82	85	•	89207	3	162244	2	
1368.841	73054.49	84		100468	4	173522	3	?
1367.563	73122.79	86		66119	1	139242	2	
1366.638	73172.27	83		83977	2	157149	2	
1361.577	73444.27	87		58243	4	131688	3	
1361.456	73450.78	65		78137	2	151587	2	
1361.224	73463.27	84		78361	4	151824	5	
				100468	4	173932	4	
1360.844	73483.79	81		103293	3	176777	4	
1360.408	73507.36	86		68891	3	142398	3	
1360.318	73512.25	35		92638	3	166151	2	
1359.282	73568.24	84		66119	1	139687	1	
				92583	2	166151	2	
1358.357	73618.33	84		63765	3	137383	2	
1357.778	73649.76	65		79444	1	153094	2	
1357.257	73678.00	60		102513	2	176190	2	
1352.666	73928.06	85		78361	4	152289	3	
1352.128	73957.49	65		92638	3	166596	4	
1351.448	73994.68	30		78361	4	152356	4	
1350.481	74047.70	25		95102	1	169149	1	
1350.080	74069.71	79	•	103293	3	177362	3	wS
1348.577	74152.22	82		78137	2	152289	3	
1346.907	74244.19	50		85798	4	160042	3	
1345.445	74324.86	83		75093	5	149418	6	
				97092	5	171417	5	
1345.097	74344.10	70	•	89803	1	164146	2	
1344.431	74380.90	60		83977	3	158358	3	+III
1343.968	74406.56	85		75819	3	150226	2	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1341.469	74545.13	83		67853	4	142398	3	
1340.776	74583.69	83		64658	2	139242	2	
1339.994	74627.23	75		103293	3	177920	2	
1339.544	74652.24	84		89582	2	164234	1	
1339.423	74659.02	85		85107	5	159766	6	d
1338.120	74731.71	70		85798	4	160529	4	
1337.985	74739.24	20		92583	2	167322	1	
1334.952	74909.05	80		75819	3	150728	4	?
1334.401	74939.99	40		89207	3	164146	2	
1334.095	74957.19	65		78137	2	153094	2	
1333.622	74983.79	85		85798	4	160781	5	d
			*	102939	1	177920	2	
1331.399	75108.94	84		67289	2	142398	3	
1330.592	75154.53	87		58243	4	133398	3	S
1330.465	75161.71	86		75819	3	150981	3	
1328.069	75297.32	72	*	95882	4	171180	3	
1327.996	75301.42	64		75093	5	150395	5	
1326.121	75407.92	86		102513	2	177920	2	+III
1325.877	75421.80	68		85107	5	160529	4	
1324.904	75477.18	84		63765	3	139242	2	
1323.894	75534.77	83		95882	4	171417	5	
1323.088	75580.79	82		67853	4	143434	5	
1322.134	75635.29	82		75093	5	150728	4	
1321.598	75665.98	83		79506	2	155174	1	
1321.466	75673.52	86	*	85107	5	160781	5	
1320.487	75729.63	53		79444	1	155174	1	
1320.162	75748.28	61		83574	0	159323	1	
1319.813	75768.32	70		75819	3	151587	2	S
1319.597	75780.72	84		97092	5	172873	4	
1319.318	75796.75	88		58243	4	134040	4	
1318.775	75827.93	79		68891	3	144719	3	
1318.488	75844.47	81		79444	1	155289	2	
1318.288	75855.95	1	*	92638	3	168495	3	
1317.325	75911.39	B1	*	92583	2	168495	3	?
1314.666	76064.97	56		83977	3	160042	2,3	
1309.807	76347.15	80		89803	1	166151	2	
1307.713	76469.39	1		75819	3	152289	3	
1306.562	76536.73	88		75819	3	152356	4	
1306.474	76541.90	79		78137	2	154678	3	
1306.032	76567.80	84	*	92583	2	169149	1	4
1306.032	76567.80	84	*	89582	2	166151	2	4
1303.268	76730.16	81		75093	5	151824	5	
1301.400	76840.34	76		97092	5	173932	4	
1300.969	76865.80	89		67853	4	144719	3	
1300.505	76893.22	1		100468	4	177362	3	

Table I.A. *(continued)*

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1299.642	76944.27	38		89207	3	166151	2	
1298.927	76986.63	89		95882	4	172873	4	+Si III
1298.073	77037.26	83		78137	2	155174	1	
1296.572	77126.47	60		103293	3	180420	2	
1296.140	77152.16	86		78137	2	155289	2	
1294.992	77220.58	87	•	68891	3	146113	4	d
1294.091	77274.31	89		75819	3	153094	2	
1292.163	77389.61	83	•	89207	3	166596	4	
1291.556	77426.00	55	*	85798	4	163225	5	
1291.490	77429.98	81		67289	2	144719	3	
1290.654	77480.12	83		102939	1	180420	2	
1289.880	77526.62	71		91623	2	169149	1	
1287.995	77640.04	84		95882	4	173522	3	
1287.948	77642.91	86		79506	2	157149	2	
1287.409	77675.40	84		79506	2	157182	1	
1287.185	77688.90	85		83574	0	161263	1	
1286.918	77705.04	82		79444	1	157149	2	
1286.658	77720.72	1		92638	3	170359	2	
1286.339	77740.03	87		89582	2	167322	1	
				64658	2	142398	3	
1285.743	77776.05	82		92583	2	170359	2	
1284.670	77841.00	84		67289	2	145130	1	
1283.575	77907.38	58		102513	2	180420	2	
1281.334	78043.67	69		95102	1	173146	2	
1280.126	78117.29	82		85107	5	163225	5	
1279.102	78179.86	86		85107	5	163287	4	
1277.801	78259.43	82		67853	4	146113	4	
1274.335	78472.31	71		92583	2	171055	3	
1272.305	78597.52	70		92583	2	171180	3	S
1271.958	78618.97	85		72968	1	151587	2	
1271.729	78633.09	85		63765	3	142398	3	
1271.641	78638.54	85		78361	4	157000	3	
1271.374	78655.08	82		103293	3	181948	2	
1270.808	78690.12	50		102513	2	181203	1	
1268.207	78851.46	59		79506	2	158358	3	
1268.092	78858.63	86		75819	3	154678	3	
1268.025	78862.80	82		78137	2	157000	3	
1267.218	78913.02	71		89582	2	168495	3	
1265.649	79010.84	84		66119	1	145130	1	w
				102939	1	181948	2	
1265.649	79010.84	84		78137	2	157149	2	
1265.101	79045.07	81		78137	2	157182	1	
1262.867	79184.89	1		102513	2	181697	3	
1260.870	79310.30	56		83977	3	163287	4	
1260.814	79313.88	1		72968	1	152282	1	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1260.302	79346.06	82		89803	1	169149	1	
1259.401	79402.86	55		79444	1	158847	2	
1258.930	79432.56	85		91623	2	171055	3	
1258.887	79435.27	81		102513	2	181948	2	
1258.350	79469.13	83		75819	3	155289	2	
1254.912	79686.84	73		78361	4	158048	4	
1252.880	79816.08	73		79506	2	159323	1	
1251.907	79878.17	81		79444	1	159323	1	
1249.055	80060.53	81		64658	2	144719	3	
1248.052	80124.86	81		72968	1	153094	2	
1247.605	80153.56	37		89207	3	169360	4	
1247.357	80169.54	76		83977	3	164146	2	
1246.012	80256.03	5		83977	3	164233	3	
1245.311	80301.21	88		58243	4	138545	5	
1244.327	80364.72	3		95102	1	175467	1	
1242.135	80506.53	5	•	92638	3	173146	2	
1241.695	80535.09	83		79506	2	160042	2,3	
1241.377	80555.73	75		89803	1	170359	2	
1241.275	80562.31	43		92583	2	173146	2	
1240.739	80597.15	81		79444	1	160042	2	
1239.794	80658.59	86	•	83574	0	164234	1	
1239.198	80697.37	1		100468	4	181166	4	
1238.993	80710.68	82		78137	2	158847	2	
1237.984	80776.52	20		89582	2	170359	2	
1237.658	80797.79	83		85798	4	166596	4	
1236.353	80883.05	82		92638	3	173522	3	
1236.178	80894.52	80		95882	4	176777	4	
1235.686	80926.73	81		68891	3	149818	4	
1235.502	80938.79	84		92583	2	173522	3	
1235.276	80953.56	55		63765	3	144719	3	
1233.224	81088.29	80		95102	1	176190	2	
1231.885	81176.42	55		92583	2	173759	1	
1230.104	81293.91	20		92638	3	173932	4	
1229.562	81329.80	84		75819	3	157149	2	
1229.487	81334.75	50		68891	3	150226	2	
[1228.34]	[81410.2]	B1		68891	3	150301	3	
1228.308	81412.83	87	*	97092	5	178505	6	w
1227.390	81473.70	82		89582	2	171055	3	
1227.302	81479.56	68		95882	4	177362	3	
1226.661	81522.13	82		91623	2	173146	2	
1225.521	81597.98	81		89582	2	171180	3	
1224.271	81681.24	77		78361	4	160042	3	
1223.503	81732.52	84		79506	2	161239	3	
1223.133	81757.23	82		79506	2	161263	1	
1222.205	81819.36	82		79444	1	161263	1	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1222.205	81819.36	B1		81404	6	163225	5	
1221.932	81837.63	83		68891	3	150728	4	
1221.762	81849.02	66		89207	3	171055	3	
1221.015	81899.10	50		91623	2	173522	3	
1220.925	81905.12	84		78137	2	160042	3	
1220.695	81920.56	79		100468	4	182389	5	
1220.035	81964.85	79		67853	4	149818	4	
1219.914	81973.03	71		89207	3	171180	3	
1218.539	82065.52	87		58243	4	140309	4	
1218.165	82090.69	83		68891	3	150981	3	
1218.165	82090.69	B1		103293	3	185384	4	
1217.499	82135.59	71		91623	2	173759	1	
1217.015	82168.27	85		78361	4	160529	4	
1216.939	82173.38	42		83977	3	166151	2	
1216.470	82205.09	65		72968	1	155174	1	
1216.118	82228.88	86		75819	3	158048	4	
1214.769	82320.15	1		72968	1	155289	2	
1214.362	82347.74	81		63765	3	146113	4	
1213.290	82420.52	83		78361	4	160781	5	
1213.113	82432.56	59		103293	3	185725	2	
1212.886	82447.98	83		67853	4	150301	3	
1211.513	82541.44	85		67853	4	150395	5	
1210.656	82599.82	86		85798	4	168397	5	
1210.377	82618.88	85		83977	3	166596	4	
1209.229	82697.31	59		85798	4	168495	3	
1208.638	82737.76	75		79506	2	162244	2	
1208.572	82742.30	78		51297	5	134040	4	
1207.934	82785.95	85		102939	1	185725	2	
1207.729	82800.01	51		79444	1	162244	2	
1206.626	82875.73	89		67853	4	150728	4	
1206.507	82883.93	93		92583	2	175467	1	+Si III
1205.735	82936.95	75		67289	2	150226	2	
1204.642	83012.23	1		67289	2	150301	3	
1204.413	83028.03	25		75819	3	158847	2	
1203.336	83102.30	68		78137	2	161239	3	
1202.958	83128.43	50		67853	4	150981	5	
1201.732	83213.23	30	•	102513	2	185725	2	p
[1200.65]	[83288.1]	B1		103293	3	186581	3	
1200.617	83290.48	84		85107	5	168397	5	
1199.863	83342.84	77		89803	1	173146	2	
1198.111	83464.74	83		68891	3	152356	4	
1196.690	83563.85	81		89582	2	173146	2	
1196.188	83598.89	69		102939	1	186538	1	
1196.069	83607.23	78		92583	2	176190	2	
1195.226	83666.20	81		89207	3	172873	4	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1194.854	83692.26	84		67289	2	150981	3	
1194.067	83747.41	52		83574	0	167322	1	
1192.690	83844.07	84		91623	2	175467	1	
1191.101	83955.91	71		89803	1	173759	1	
1190.889	83970.87	89		67853	4	151824	5	
1189.499	84068.98	84		102513	2	186581	3	
1189.432	84073.73	75		97092	5	181166	4	
1188.962	84106.98	85		66119	1	150226	2	
1188.668	84127.79	74		103293	3	187421	2	
1188.517	84138.50	85		92638	3	176777	4	
1188.284	84154.95	3		58243	4	142398	3	
1187.926	84180.32	79		72968	1	157149	2	
1187.610	84202.77	78		68891	3	153094	2	
1187.453	84213.88	25		72968	1	157182	1	
				95102	1	179316	1	
1187.335	84222.23	73		75819	3	160042	3	
1186.901	84253.01	84		85107	5	169360	4	
1186.262	84298.43	85		67289	2	151587	2	
1186.030	84314.90	82		89207	3	173522	3	
1184.749	84406.09	84		85107	5	169513	6	
1184.339	84435.28	87		67853	4	152289	3	?
1183.679	84482.41	5	*	102939	1	187421	2	
1183.423	84500.67	82	•	67853	4	152356	4	?
1183.179	84518.10	83		83977	3	168495	3	
1182.487	84567.50	32		91623	2	176190	2	
1181.475	84639.97	70		79506	2	164146	2	
1181.024	84672.27	89		75093	5	159766	6	
1180.606	84702.26	70		79444	1	164146	2	
1180.284	84725.38	86		89207	3	173932	4	
			*	92638	3	177362	3	
1179.538	84778.94	60		92583	2	177362	3	
1179.378	84790.43	5	•	79444	1	164234	1	
1178.362	84863.56	82		78361	4	163225	5	
1177.742	84908.24	60		102513	2	187421	2	
1177.648	84915.06	80		100468	4	185384	4	
1177.496	84925.96	60		78361	4	163287	4	
1177.006	84961.31	84		100468	4	185430	5	
[1176.47]	[84999.8]	B1		67289	2	152289	3	+II
1176.562	84993.41	74		67289	2	152282	1	
1175.885	85042.35	75		103293	3	188335	3	
1173.844	85190.18	83		58243	4	143434	5	
1173.267	85232.09	30		103293	3	188525	2	S
1172.918	85257.48	60		85798	4	171055	3	
1172.558	85283.63	85		95882	4	181166	4	
1172.373	85297.08	84		97092	5	182389	5	

Table I.A. *(continued)*

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1172.093	85317.45	80		95102	1	180420	2	
1171.822	85337.22	25		92583	2	177920	2	
1171.191	85383.14	50		85798	4	171180	3	
				83977	3	169360	4	
1170.678	85420.58	81		75819	3	161239	3	
1170.468	85435.89	84		75093	5	160529	4	
1168.668	85567.50	83		64658	2	150226	2	
1168.415	85586.01	5		102939	1	188525	2	
1167.964	85619.10	77		85798	4	171417	5	
1167.635	85643.19	84		64658	2	150301	3	
1167.358	85663.56	78		89803	1	175467	1	
1167.023	85688.12	87		75093	5	160781	5	
1166.330	85739.01	70		91623	2	177362	3	
1165.680	85786.81	30		68891	3	154678	3	
1165.436	85804.77	58		67289	2	153094	2	
1165.289	85815.63	79		95882	4	181697	3	
1164.531	85871.51	84		78361	4	164233	3	
1164.351	85884.80	69		89582	2	175467	1	
1162.626	86012.20	71		102513	2	188525	2	
1162.074	86053.02	84		63765	3	149818	4	
1161.485	86096.71	77		78137	2	164233	3	
				78137	2	164234	1	
1161.270	86112.61	17		100468	4	186581	3	
1160.588	86163.20	82		66119	1	152282	1	
1158.784	86297.36	60		91623	2	177920	2	
1158.620	86309.56	86		85107	5	171417	5	
1158.440	86322.98	76		64658	2	150981	3	
1158.020	86354.27	79		72968	1	159323	1	
1157.651	86381.85	80		83977	3	170359	2	
1157.577	86387.32	30		89803	1	176190	2	
1157.429	86398.38	76	*	68891	3	155289	2	
1157.080	86424.48	55		75819	3	162244	2	
1156.594	86460.73	82		63765	3	150226	2	
1156.396	86475.55	86		58243	4	144719	3	
1155.970	86507.41	79		95882	4	182389	5	
1155.585	86536.26	84		63765	3	150301	3	
1153.320	86706.23	72		79444	1	166151	2	
1152.962	86733.10	60		92583	2	179316	1	
1151.746	86824.74	30		67853	4	154678	3	S
1150.361	86929.26	46		64658	2	151587	2	
1149.907	86963.58	76		63765	3	150728	4	
1149.760	86974.67	75		66119	1	153094	2	
1149.642	86983.64	25		89207	3	176190	2	
1148.452	87073.74	80		72968	1	160042	2	
1148.391	87078.36	76		83977	3	171055	3	

Table I.A. (*continued*)

λ (Å)	σ (cm⁻¹)	Int		E_{even}	J_e	E_{odd}	J_0	Note
1146.754	87202.63	58		83977	3	171180	3	
1146.580	87215.92	79		63765	3	150981	3	
1146.152	87248.45	87		51297	5	138545	5	
1145.450	87301.94	73		103293	3	190595	3	
1143.278	87467.77	5		75819	3	163287	4	
1141.232	87624.61	74		64658	2	152282	1	
1141.157	87630.36	79		64658	2	152289	3	
1139.944	87723.61	42		85798	4	173522	3	
1139.537	87754.96	89		51297	5	139051	6	
1139.413	87764.52	66		85107	5	172873	4	
1139.210	87780.14	67		89582	2	177362	3	
[1138.66]	[87822.3]	Bl		63765	3	151587	2	+II
1138.476	87836.74	44		92583	2	180420	2	
1138.054	87869.32	83		58243	4	146113	4	
1136.156	88016.06	60	*	78137	2	166151	2	d
1134.952	88109.47	86		81404	6	169513	6	
1134.855	88116.98	23		89803	1	177920	2	
[1134.63]	[88134.4]	Bl		85798	4	173932	4	
1134.662	88132.00	86		75093	5	163225	5	
1134.361	88155.30	64		89207	3	177362	3	?
1133.340	88234.77	72		78361	4	166596	4	
1133.042	88257.98	70		68891	3	157149	2	
1132.571	88294.70	1		72968	1	161263	1	
1132.015	88338.02	77		97092	5	185430	5	
				89582	2	177920	2	
1131.050	88413.40	40		75819	3	164233	3	
1130.762	88435.97	83		64658	2	153094	2	
1129.638	88523.91	80		63765	3	152289	3	
1129.591	88527.59	70		92638	3	181166	4	
1128.790	88590.42	85		63765	3	152356	4	
1127.224	88713.55	21		89207	3	177920	2	
1126.167	88796.82	29		91623	2	180420	2	
1125.809	88825.00	62		85107	5	173932	4	
1123.441	89012.27	83		51297	5	140309	4	
1122.906	89054.64	74		66119	1	155174	1	
1122.848	89059.28	30		92638	3	181697	3	
1222.152	89114.48	33	*	92583	2	181697	3	w
1121.744	89146.93	53		67853	4	157000	3	
1121.614	89157.23	84		68891	3	158048	4	
1121.461	89169.38	78		83977	3	173146	2	
				66119	1	155289	2	
1121.244	89186.69	53	*	78137	2	167322	1	
1120.129	89275.40	52		72968	1	162244	2	
1119.461	89328.72	53		63765	3	153094	2	
1117.735	89466.65	50		68891	3	158358	3	

Table I.A. (*continued*)

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1114.695	89710.62	76		67289	2	157000	3	
1112.841	89860.12	5		67289	2	157149	2	
1112.434	89892.95	76		67289	2	157182	1	
1111.660	89955.60	60		83977	3	173932	4	
1110.952	90012.91	74		81404	6	171417	5	
1110.867	90019.80	78		64658	2	154678	3	
1110.660	90036.56	67		78361	4	168397	5	
1109.552	90126.46	5		100468	4	190595	3	
1109.462	90133.75	49		78361	4	168495	3	
1104.894	90506.41	68	•	67853	4	158358	3	w
1102.553	90698.63	26		95882	4	186581	3	
1098.914	90998.98	68		78361	4	169360	4	
1098.542	91029.74	39		66119	1	157149	2	
1098.076	91068.36	40		67289	2	158358	3	
1096.758	91177.79	62		72968	1	164146	2	
1092.619	91523.22	72		63765	3	155289	2	
1092.316	91548.59	4		79506	2	171055	3	
1092.009	91574.36	75		58243	4	149818	4	
1091.254	91637.68	45		68891	3	160529	4	
1086.565	92033.12	1		67289	2	159323	1	
1085.342	92136.87	71		51297	5	143434	5	
1085.173	92151.18	82		58243	4	150395	5	
1084.449	92212.77	37		83977	3	176190	2	
1082.867	92347.41	79		68891	3	161239	3	
1081.261	92484.63	54		58243	4	150728	4	
1079.037	92675.24	66		67853	4	160529	4	
1078.818	92694.01	53		78361	4	171055	3	
1078.225	92744.99	34		92638	3	185384	4	
1078.142	92752.17	74		67289	2	160042	3,2	
1077.594	92799.33	10		83977	3	176777	4	
1072.568	93234.20	67		63765	3	157000	3	
1070.683	93398.31	72		85107	5	178505	6	
1068.600	93580.41	79		58243	4	151824	5	
1063.323	94044.82	72		58243	4	152289	3	
1060.285	94314.29	1		79444	1	173759	1	
1059.851	94352.90	1		72968	1	167322	1	
1059.098	94419.99	54		75093	5	169513	6	
1055.826	94712.62	4		95882	4	190595	3	
1054.676	94815.85	70		51297	5	146113	4	
1051.723	95082.08	38		63765	3	158847	2	
1051.039	95143.93	1		66119	1	161263	1	
1049.809	95255.40	1		68891	3	164146	2	
1048.571	95367.91	47		85798	4	181166	4	
1035.145	96604.87	1		64658	2	161263	1	
1019.206	98115.54	1	*	66119	1	164234	1	

Table I.A. *(continued)*

λ (Å)	σ (cm^{-1})	Int		E_{even}	J_e	E_{odd}	J_0	Note
1015.028	98519.41	12	•	51297	5	149818	4	
1012.734	98742.66	1		67853	4	166596	4	

Notes:
- 1 perturbed by a close Au II line
- 2 blend with a line of Au II or Au III character
- 3 double line perturbed by Si II line at 1533.432Å
- 4 blend with O I line at 1306.0286Å
- +III blend with a classified line of Au III
- + II blend with a classified line of Au II
- +I blend with a classified line of Au I
- w wide line
- d double line
- p perturbed by a close line
- S intensity is too strong with regard to the calculated line strength
- ? doubtful classification
- Bl blend with another line
- * the measured wavelength and the wavelength derived from energy levels differ more than 0.010Å

Table I.B. *Additional classified lines in the $5d^8$–$5d^7 6p$ array of Au IV*

λ(Å)	σ (cm^{-1})	Int.	Char.	Even	J_e	Odd	J_o	
840.221	119 016.4	11	1	25702	4	144 719	3	
837.561	119 394.3	8	2	12293	3	131 688	1	
833.299	120 004.9	54	7	12293	3	132 300	2	
831.830	120 216.9	24	1	0	4	120 217	4	
823.029	121 502.4	21	1	18185	0	139 687	1	
816.360	122 495.0	10	2	0	4	122 495	5	
808.081	123 750.0	13	1	6630	2	130 380	2	
804.587	124 287.4	28	1	6630	2	130 918	2	
795.735	125 670.0	12	1	6630	2	132 300	2	
788.841	126 768.3	37	1	6630	2	133 398	3	
787.715	126 949.5	37	1	12293	3	139 242	2	O IV
777.678	128 587.9	5	2	30736	2	159 323	1	
759.380	131 686.3	2	2	0	4	131 688	3	
754.082	132 611.6	14	1	6630	2	139 242	2	
751.554	133 057.6	17	1	6630	2	139 687	1	
749.638	133 397.8	39	1	0	4	133 398	3	
749.566	133 410.5	4	2	30736	2	164 146	2	
721.755	138 551.1	31	1	21490	1	160 042	2	
715.443	139 773.5	29	1	21490	1	161 263	1	
708.088	141 225.3	7	2	18101	2	159 323	1	
704.519	141 940.9	51	1	18101	2	160 042	2	N
700.345	142 786.7	6	2	30736	2	173 522	3	
696.090	143 659.6	23	1	25702	4	169 360	4	
686.534	145 659.3	52	1	6630	2	152 289	3	
684.699	146 049.5	14	2	18101	2	164 146	2	D
676.492	147 821.4	11	1	25702	4	173 522	3	
667.469	149 819.7	36	1	0	4	149 818	4	S
661.915	151 076.8	10	3	25702	4	176 777	4	
658.529	151 853.6	3	2	12293	3	164 146	2	
656.640	152 290.4	23	1	0	4	152 289	3	
654.900	152 695.0	66	1	6630	2	159 323	1	N
646.683	154 635.4	19	1	6630	2	161 263	1	
638.207	156 688.9	76	1	30736	2	187 421	2	D
636.664	157 068.6	8	2	12293	3	169 360	4	
635.799	157 282.5	26	1	18185	0	175 467	1	
635.456	157 367.3	6	2	18101	2	175 467	1	
634.846	157 518.6	74	1	6620	2	164 146	2	
626.249	159 680.9	5	2	25702	4	185 384	4	
621.961	160 781.9	63	1	0	4	160 781	5	
602.665	165 929.8	11	2	21490	1	187 421	2	
592.172	168 870.0	12	1	12293	3	181 166	4	
590.612	169 315.9	1	2	18101	2	187 421	2	
573.762	174 288.3	2	2	12293	3	186 582	3	

Notes: O IV, blend with O IV line at 787.711 Å; D, blend with a transition reported in [1]; S, much stronger than expected; N, revised classification.

Char: 1, normal line; 2, diffuse line; 3, very diffuse, doubtful; 7, line on shoulder of another line.

Table II. *Oscillator strengths of selected strong lines of Au IV*

Wavelength (Å)	Lower level (cm^{-1})	J	gf
1909.700	67 853	4	0.128
1830.087	67 853	4	0.483
1809.560	78 137	2	0.139
1717.612	75 819	3	0.526
1554.946	85 107	5	3.01
1536.725	78 361	4	2.26
1450.953	51 297	5	2.76
1449.470	81 404	6	2.58
1404.525	51 297	5	2.36
1245.311	58 243	4	2.04
1228.308	97 092	5	5.72
1217.015	78 361	4	2.16
1216.118	75 819	3	2.23
1210.656	85 798	4	3.12
1190.889	67 853	4	2.70
	81 404	6	7.20 *
1189.499	102 513	2	2.67
1188.517	92 638	3	2.80
1181.024	75 093	5	5.77
1177.648	100 468	4	2.42
1177.006	100 468	4	4.31
1172.558	95 882	4	2.79
1172.373	97 092	5	3.17
1158.620	85 107	5	3.41
1146.152	51 297	5	2.53
1139.537	51 297	5	6.51
1134.952	81 404	6	4.65
1128.790	63 765	3	2.22

* Inasmuch as the classification 81 404 (6)–165 375 (7) is also valid for λ1190.889 Å.

Table III. *Energy levels of $5d^8 + 5d^7 6s(+5d^6 6s^2)$ in Au IV. Experimental energies E_{exp}, theoretical energies, E_{th} and $\Delta E = E_{exp} - E_{th}$ are in cm^{-1}. The first LS component and the amount of the three configurations in the eigenfunction are given in percents*

E_{exp}	E_{th}	ΔE	Lead. comp. %		d^8 %	$d^7 s$ %	$d^6 s^2$ %
$J = 0$							
18185.5	18194	−9	$d^8\,{}^3P$	82	97.9	1.8	0.3
	55369		$d^8\,{}^1S$	83	97.9	1.7	0.4
83574.79	83574	1	$({}^2P)\,{}^3P$	58	2.7	96.8	0.6
	97316		$({}^4P)\,{}^3P$	58	1.0	96.0	3.0
$J = 1$							
21490.1	21482	8	$d^8\,{}^3P$	97	97.0	2.8	0.2
66119.69	66133	−14	$({}^4F)\,{}^5F$	46	0.5	99.3	0.1
72968.97	72947	22	$({}^4P)\,{}^5P$	48	0.8	99.1	0.1
79444.72	79472	−27	$({}^2P)\,{}^1P$	32	0	99.5	0.5
89803.45	89787	17	$({}^4P)\,{}^3P$	31	0.6	97.6	1.8
95102.32	95106	−4	$({}^2P)\,{}^3P$	40	0.8	98.7	0.5
102939.66	102972	−33	$({}^2P)\,{}^1P$	37	0	99.1	0.9
	116800		$(1\,{}^2D)\,{}^3D$	82	0	99.5	0.5
$J = 2$							
6630.0	6636	−6	$d^8\,{}^1D$	46	98.2	1.6	0.2
18101.3	18105	−4	$d^8\,{}^3P$	48	98.1	1.7	0.2
30736.0	30727	9	$d^8\,{}^1D$	49	98.1	1.7	0.2
64658.73	64636	22	$({}^4F)\,{}^5F$	30	1.3	98.2	0.4
67289.50	67260	30	$({}^4F)\,{}^5F$	39	0.5	99.4	0.1
78137.00	78137	0	$({}^4F)\,{}^3F$	45	0.6	98.7	0.8
79506.82	79491	16	$({}^4P)\,{}^3P$	56	0.4	97.6	2.1
89582.20	89602	−19	$({}^4P)\,{}^3P$	30	0.3	98.9	0.8
91623.26	91637	−13	$({}^2F)\,{}^3F$	80	0.6	98.2	1.3
92583.10	92576	7	$(3\,{}^2D)\,{}^3D$	22	0.7	98.4	1.0
102513.10	102475	38	$(3\,{}^2D)\,{}^1D$	34	0.7	97.0	2.3
	117697		$(1\,{}^2D)\,{}^3D$	72	0.2	98.9	1.0
	123390		$(1\,{}^2D)\,{}^1D$	72	0.0	96.7	3.3
$J = 3$							
12293.5	12317	−23	$d^8\,{}^3F$	99	99.4	0.5	0.2
63765.62	63768	−3	$({}^4F)\,{}^5F$	68	0.0	99.9	0.0
68891.56	68908	−17	$({}^4P)\,{}^5P$	66	0.0	99.9	0.1
75819.70	75821	−1	$({}^4F)\,{}^3F$	58	0.0	99.4	0.6
83977.35	83998	−20	$({}^2G)\,{}^3G$	74	0.1	99.5	0.5
89207.08	89231	−24	$(3\,{}^2D)\,{}^3D$	46	0.0	99.5	0.5
92638.62	92660	−21	$({}^2F)\,{}^3F$	65	0.3	98.9	0.8
103293.45	103284	10	$({}^2F)\,{}^1F$	66	0.1	97.9	2.0
	118877		$(1\,{}^2D)\,{}^3D$	65	0.0	98.6	1.4
$J = 4$							
0.0	−21	21	$d^8\,{}^3F$	95	99.5	0.3	0.1
25702.4	25700	2	$d^8\,{}^1G$	94	98.4	1.5	0.2
58243.84	58237	6	$({}^4F)\,{}^5F$	66	0.2	99.7	0.1
67853.56	67858	−5	$({}^4F)\,{}^3F$	50	0.1	99.3	0.4
78361.38	78360	1	$({}^2G)\,{}^3G$	37	0.3	99.6	0.3
85798.00	85762	36	$({}^2G)\,{}^1G$	35	0.6	98.4	1.0
95882.34	95883	0	$({}^2H)\,{}^3H$	50	0.3	99.1	0.6
100468.80	100455	15	$({}^2F)\,{}^3F$	63	0.4	98.8	0.9
$J = 5$							
51297.15	51306	−9	$({}^4F)\,{}^5F$	86	0.0	100.0	0.0
75093.64	75101	−8	$({}^2G)\,{}^3G$	60	0.0	99.8	0.2
85107.45	85106	2	$({}^2H)\,{}^3H$	56	0.0	99.8	0.2
97092.09	97085	7	$({}^2H)\,{}^1H$	59	0.0	99.7	0.3
$J = 6$							
81404.23	81414	−10	$({}^2H)\,{}^3H$	100	0.0	99.8	0.2

Table IV. *Energy levels of $5d^7 6p$ in Au IV. Experimental energies E_{exp}, theoretical energies E_{th} and $\Delta E = E_{exp} - E_{th}$ are in cm^{-1}. The first LS component and the amount of $5d^7 6p$ in the eigenfunction are given in percents. N and R denote new and revised levels respectively*

	E_{exp}	E_{th}	ΔE	1st comp.	%	d^7p %
$J = 0$						
		141 001		$^4P\,^5D$	55	98.2
		149 991		$^2P\,^1S$	37	97.4
		158 519		$^2P\,^3P$	55	98.3
		162 614		$^4F\,^5D$	54	96.5
		176 394		$^4P\,^3P$	57	96.7
		182 978		$3^2D\,^3P$	59	96.4
		202 829		$1^2D\,^3P$	70	95.6
$J = 1$						
N	130 380.64	130 534	−153	$^2P\,^3P$	22	98.0
N	139 687.91	139 917	−229	$^4F\,^5F$	28	98.2
	145 130.75	145 002	129	$^4P\,^5D$	22	98.2
	152 282.98	152 302	−17	$^4F\,^5D$	33	97.1
	155 174.17	155 023	151	$^4F\,^5F$	25	97.6
	157 182.27	157 678	−496	$^4F\,^3D$	21	97.3
N	159 323.09	159 490	−166	$^2P\,^1P$	23	96.9
N	161 263.80	161 369	−105	$^2P\,^3D$	24	96.7
	164 234.15	164 485	−251	$^4F\,^3D$	21	97.6
	167 322.20	167 361	−37	$^4P\,^3S$	18	97.8
	169 149.98	168 930	217	$3^2D\,^3D$	26	97.3
	173 759.39	173 534	226	$3^2D\,^3P$	16	97.0
N	175 467.30	175 320	148	$3^2D\,^3P$	19	96.1
	179 316.21	179 191	126	$^2F\,^3D$	46	96.5
	181 203.21	181 078	127	$^2P\,^3S$	33	96.8
	186 538.60	186 747	−208	$^2P\,^1P$	19	97.7
		191 045		$1^2D\,^3D$	44	95.4
		201 068		$1^2D\,^3P$	57	95.0
		208 397		$1^2D\,^1P$	53	96.5
$J = 2$						
N	130 918.01	131 029	−111	$^2P\,^3D$	15	98.0
N	132 300.53	132 508	−208	$^4F\,^5F$	16	98.1
N	137 383.91	137 724	−341	$^4P\,^5S$	34	97.9
N	139 242.63	139 422	−180	$^4F\,^5G$	35	98.4
	150 226.36	150 238	−11	$^2P\,^3P$	21	97.5
	151 587.94	151 514	75	$^4F\,^5D$	13	97.9
	153 094.36	153 146	−51	$3^2D\,^3P$	18	97.3
	155 289.09	155 535	−245	$^4F\,^5F$	19	97.6
	157 149.66	157 278	−126	$^4F\,^3F$	15	97.3
	158 847.64	158 829	19	$^2F\,^3F$	18	97.7
N	160 042.25	159 923	119	$^4P\,^3P$	21	97.3
	162 244.52	162 057	189	$^4F\,^3D$	34	97.8
N	164 146.91	164 271	−124	$3^2D\,^3F$	15	96.8
	166 151.09	166 114	38	$^2P\,^3D$	23	98.0
	170 359.28	170 207	153	$^2G\,^3F$	30	97.3
	173 146.00	173 214	−70	$^2F\,^3D$	15	97.0
	176 190.77	176 119	72	$^2P\,^3D$	23	97.1
	177 920.75	178 152	−230	$3^2D\,^3P$	10	97.1
	180 420.20	180 600	−177	$^2P\,^1D$	22	96.5
	181 948.41	181 860	88	$^2F\,^3D$	21	96.9
	185 725.60	185 917	−190	$1^2D\,^3F$	33	97.3
N	187 421.30	187 467	−46	$1^2D\,^3P$	35	96.0
	188 525.60	188 234	290	$1^2D\,^3F$	22	96.2
		202 929		$1^2D\,^3D$	57	95.7
		206061		$1^2D\,^1D$	39	93.3
$J = 3$						
N	131 688.08	131 788	−100	$^4F\,^5D$	36	98.4
N	133 398.58	133 495	−96	$^4F\,^5G$	28	98.6
	142 398.70	142 031	368	$^4P\,^5D$	26	98.1
	144 719.33	144 920	−200	$^4F\,^3D$	50	97.6
	150 301.72	149 990	313	$^4F\,^5D$	29	98.2
	150 981.66	150 930	52	$^2G\,^1F$	15	97.5
R	152 289.28	152 414	−125	$^2F\,^3G$	16	97.2
	154 678.44	154 758	−78	$3^2D\,^3D$	20	98.3
	157 000.22	156 904	96	$^2F\,^3G$	24	98.1
	158 358.19	158 402	−44	$^4F\,^3F$	35	97.9
	160 042.25	160 191	−149	$^4F\,^3G$	35	97.6
	161 239.56	161 178	61	$^4P\,^3D$	33	96.2
	164 233.10	164 166	71	$^2G\,^3F$	25	97.8
	168 495.28	168 301	198	$^2G\,^3G$	36	97.5
	171 055.81	170 961	94	$^2G\,^1F$	20	97.6
	171 180.59	171 117	65	$^4P\,^5D$	11	97.4
N	173 522.09	173 391	131	$^2F\,^3F$	20	96.8
	177 362.38	177 243	121	$^2F\,^3F$	16	96.7
	181 697.94	181 800	−100	$^2H\,^3G$	34	97.4
	186 581.60	186 672	−91	$3^2D\,^3F$	23	95.8
	188 335.80	187 869	466	$^2F\,^1F$	48	97.9
N	190 595.20	190 689	−94	$^2F\,^1F$	13	75.4
		203 678		$1^2D\,^1F$	38	96.1
		208 423		$1^2D\,^3D$	47	94.0
$J = 4$						
N	120 217.71	120 172	45	$^4F\,^5D$	42	98.4
	134 040.04	133 983	56	$^4F\,^5G$	44	98.9
	140 309.22	140 314	−5	$^4F\,^5D$	33	98.0
	146 113.06	145 843	271	$^4F\,^3F$	30	98.8
R	149 818.39	149 925	−106	$^2G\,^3H$	34	98.2
	150 728.91	150 724	6	$^4F\,^5F$	27	98.5
	152 356.19	152 374	−16	$^4P\,^5D$	31	97.9
	158 048.39	158 040	9	$^4P\,^5D$	47	97.5
	160 529.44	160 306	225	$^2G\,^3F$	26	97.6
	163 287.55	163 395	−109	$^2H\,^3G$	41	98.8
	166 596.09	166 417	177	$^2G\,^3G$	28	97.8
N	169 360.63	169 363	−2	$^2H\,^1G$	24	96.9
	172 873.20	172 999	−126	$3^2D\,^3F$	21	97.7
	173 932.41	174 197	−264	$3^2D\,^3F$	30	97.7
N	176 777.16	176 868	−91	$^2F\,^1G$	39	96.6
N	181 166.03	181 071	95	$^2H\,^3H$	43	97.0
N	185 384.00	185 282	101	$^2F\,^3F$	50	93.8
		202 647		$1^2D\,^3F$	63	95.0
$J = 5$						
N	122 495.59	122 132	363	$^4F\,^5F$	30	98.9
	138 545.13	138 276	268	$^4F\,^5F$	54	98.6
	143 434.33	143 474	−40	$^2H\,^3I$	22	98.8
N	150 395.02	150 178	217	$^2H\,^3G$	56	98.8
	151 824.27	151 748	75	$^4F\,^5G$	48	99.1
N	160 781.77	160 882	−100	$^2H\,^3I$	46	98.7
	163 225.23	163 392	−168	$^2H\,^3H$	23	98.5
	168 397.94	168 638	−244	$^2G\,^1H$	36	98.4
	171 417.08	171 266	150	$^2H\,^1H$	33	97.2
	182 389.57	182 587	−197	$^2H\,^1H$	32	97.2
N	185 430.11	185 386	45	$^2F\,^3G$	48	95.8
$J = 6$						
N	139 051.75	138 836	215	$^4F\,^5G$	80	99.4
N	149 418.33	149 478	−60	$^2H\,^3I$	47	99.1
N	159 766.00	159 821	−55	$^2G\,^3H$	52	98.9
N	169 513.47	169 468	46	$^2H\,^3H$	78	97.8
N	178 505.76	178 785	−279	$^2H\,^3I$	34	98.7
$J = 7$						
?	165 375.10	165 426		$^2H\,^3I$	99	99.5

Table V. *Energy parameters for* $5d^76p + 5d^66s6p + 5d^56s^26p$. *Fitted values and ab initio integrals determined by the HXR method for* $5d^76p$ *are used to scale ab initio integrals for* $5d^66s6p$ *and* $5d^56s^26p$. *The rms deviation is 185* cm^{-1}

Parameters for $5d^76p$	Fitted	st. dev.	HXR	
$F^2(5d,5d)$	60097	531	62976	
$F^4(5d,5d)$	44253	625	42020	
$F^2(5d,6p)$	23967	384	26924	
$G^1(5d,6p)$	8452	115	10097	
$G^3(5d,6p)$	9079	468	8741	
ζ_{5d}	5979	24	5919	
ζ_{6p}	11799	55	12848	
Parameters for $5d^66s6p$				
$F^2(5d,5d)$	61509		64388	
$F^4(5d,5d)$	45293		43095	
$F^2(5d,6p)$	24597		27630	
$G^1(5d,6p)$	8393		10025	
$G^3(5d,6p)$	9130		8791	
$G^2(5d,6s)$	20966		18635	
$G^1(6s,6p)$	35776		40500	
ζ_{5d}	6271		6208	
ζ_{6p}	12548		13665	
Parameters for $5d^56s^26p$				
$F^2(5d,5d)$	62922		65765	
$F^4(5d,5d)$	46333		44126	
$F^2(5d,6p)$	25198		28307	
$G^1(5d,6p)$	8325		9950	
$G^3(5d,6p)$	9173		8833	
ζ_{5d}	6568		6503	
ζ_{6p}	13309		14492	
Configuration interaction				
$\alpha(5d,5d)$	58			
$\beta(5d,5d)$	290	94		
$\alpha(5d,6p)$	−43	7		
$R^2(5d5d,6s6s)$	22231	r	25475	$5d^76p$–$5d^56s^26p$
$R^2(5d5d,5d6s)$	−24546	1043	−28127	$5d^76p$–$5d^66s6p$
$R^2(5d5d,5d6s)$	−24432	r	−27998	$5d^66s6p$–$5d^56s^26p$
$R^2(5d6p,6s6p)$	−21704	r	−24871	$5d^76p$–$5d^66s6p$
$R^2(5d6p,6s6p)$	−21832	r	−25017	$5d^66s6p$–$5d^56s^26p$
$R^1(5d6p,6p6s)$	−18981	r	−21751	$5d^76p$–$5d^66s6p$
$R^1(5d6p,6p6s)$	−18871	r	−21624	$5d^66s6p$–$5d^56s^26p$

Note: r, all seven Slater parameter for configuration interaction have the same scaling factor.