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Revised and Extended Analyses of the Pd-Like Ion Spectra Sb VI, Te VII and I VIII

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Abstract

The $4d^95l - 4d^95l'$ transitions in the Pd-like ion spectra Sb VI, Te VII and I VIII have been reinvestigated in the $400 - 900 \text{ \AA}$ wavelength region using vacuum spark sources. In Sb VI and Te VII, the previous analyses of the $4d^95s - 4d^95p$ and $4d^95p - 4d^95d$ transitions have been extended by respectively six and twenty-six newly classified lines. An additional forty-four and forty-nine lines have been identified as $4d^95d - 4d^95f$ transitions leading to the determination of the $4d^95f$ levels in Sb VI and Te VII. For I VIII, the previously identified $4d^95s - 4d^95p$ transitions have been remeasured and seven new lines were added. The $4d^95s$ and $4d^95p$ level energies have been revised. An additional forty-seven lines have been identified as $4d^95p - 4d^95d$ transitions leading to the determination of the $4d^95d$ levels. Resonance lines have been remeasured for Te VII and I VIII in the grazing incidence region. The $4d^95d$ 1S_0 levels, of crucial interest in the development of X-UV lasers, have been established for the first time in all three spectra studied.

1. Introduction

The $4d^95p$ $^1P_1 - 4d^95d$ 1S_0 and $4d^95d$ $^1P_1 - 4d^95f$ 1P_1 transitions in the Pd-like ions are perspectives for the laser effect in the extreme ultraviolet spectral region [1]. For the purpose of modeling a laser medium, not only the levels involved in the laser transitions are needed but also the levels that likely enter the population kinetics. In the Pd-like ions, an extended identification of all the $4d^95l$ and of the nearby $4d^94f$ levels would be necessary to support *ab initio* calculations in a collisional – radiative model of these ions. In this respect the knowledge of the $4d^95l$ configuration energy structures of these ions is far from completeness. At the beginning of the present work, along the Pd I isoelectronic sequence, the $4d^95s$ and $4d^95p$ levels were determined up to Cs X [2–12]; the $4d^95d$ levels were known up to Te VII [3–4, 13–14] except the very important $4d^95d$ 1S_0 levels which were established only for Pd I and for Ag II [2]. As for the $4d^95f$ configuration, no level was known except the $J = 1$ ones, determined through the resonance transitions to the ground term $4d^{10}$ 1S_0 in Cd III – Cs X [12]. The strongest resonance transitions from the $4d^95p$ and $4f$ ($J = 1$) levels were identified up to Dy XXI and Ho XXII respectively [11] and extended to Pt XXXIII for some of the $4d^94f$ ($J = 1$) levels [15]. The purpose of the present work is to revise and extend the spectroscopic data for $4d^95l$ configurations in the spectra of Pd-like ions Sb VI, Te VII and I VIII, and in particular, to establish the $4d^95d$ 1S_0 level in these ions.

2. Experiment and method of analysis

The spectra of the $4d^95l - 4d^95l'$ transitions in Sb VI, Te VII and I VIII were obtained by using a 6.65 m normal incidence spectrograph at the Institute for Spectroscopy (Troitsk, Russia). The spectrograph is equipped with a 1200 1/mm grating and has a plate factor of 1.25 \AA/mm . The spectra were recorded on Ilford Q2 photographic plates. Different plasma sources were used for the ionization stage selection. For the excitation of “hot” spectra a 4 kV low-inductance vacuum spark with $10 \mu\text{F}$ capacitance was used. The peak discharge current of this source could be varied from 30 to 10 kA by using an inductance coil in series. “Cold” spectra were excited in a 1 kV sliding spark with peak currents of 2–3 kA. In both sources we used aluminum electrodes with chemically pure antimony, tellurium or potassium iodide packed into the anode.

The iodine spectrum was also photographed in the $400-800 \text{ \AA}$ region on a 10.7 m normal incidence spectrograph at the Observatoire de Meudon, equipped with a 3600 1/mm holographic grating leading to a plate factor of about 0.26 \AA/mm . This spectrum was excited in a 15 kV vacuum triggered spark with a $4.82 \mu\text{F}$ capacitance and was recorded on Kodak SWR photographic plates. The iodine spectrum obtained on this spectrograph is better resolved than the one obtained on the Troitsk spectrograph. Therefore the corresponding set of plates was used for finalizing the I VIII analysis.

The energies of the $4d^95l$ levels relative to the ground state are determined by the wavenumbers of the $4d^{10}$ $^1S_0 - 4d^95p$ and $5f$ ($J = 1$) resonance transitions. Therefore we paid particular attention to the measurement of the corresponding wavelengths, which are located in the $100-300 \text{ \AA}$ region and reported in [12]. For a re-measurement of these lines in Te VII and I VIII new spectra were obtained at Troitsk on a 3 m grazing incidence spectrograph with a 3600 1/mm holographic grating and excited in a low-inductance vacuum spark. The accurately measured wavelengths of titanium ions [17] were used as standards in this case and the estimated uncertainty of the wavelength measurements is about 0.003 \AA (For Sb VI ion we already published [12] the accurate resonance wavelengths measured by using the Ti-standards).

The spectrograms were measured on an automatic microdensitometer at Troitsk and on a semi-automatic comparator at Meudon. The lines of the O III – O V ions [16] and of the ions of lower ionization stages of the inves-

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tigated atoms were used as wavelength standards. The estimated wavelength measurement accuracy is about 0.003–0.005 Å for the unperturbed lines in the 400–1000 Å region. The line intensities measured at Troitsk on a 1–1000 scale take into account the modeled photoemulsion characteristic curve.

The spectra analyses were carried out by means of the complex spectra identification program IDEN [18] on the basis of predicted energies and transition probabilities derived from the Cowan computer codes [19]. We included into calculations the even $4d^{10}$, $4d^9ns$ ($n = 5, 6$), $4d^9nd$ ($n = 5, 6$), $4d^85s^2$, $4d^85s5d$, $4d^85d^2$ and $4p^54d^{10}5p$ con-

Table I. Identified spectral lines in Sb VI.

gA	$I(a)$	λ (Å)	σ (cm $^{-1}$)	$\Delta\sigma$	Transition
<i>5p – 5d and 5p – 6s transitions (addition to [14])</i>					
0.5	45	594.474	168216.0	0.0	5p 3D_1 357446.0 – 6s 3D_2 525662.0
0.1	35	603.364	165737.5	-1.2	5p 3P_1 341970.6 – 5d 1S_0 507709.3
0.3	87	634.301	157654.0	-1.5	5p 3P_2 331122.8 – 5d 3F_3 488778.3
10.3	449	638.160	156700.5	0.5	5p 1P_1 351009.3 – 5d 1S_0 507709.3
0.2	51	640.906	156029.1	1.7	5p 3P_2 331122.8 – 5d 3D_2 487150.2
1.9	125	665.497	150263.7	0.4	5p 3D_1 357446.0 – 5d 1S_0 507709.3
<i>5d – 5f transitions</i>					
0.2	15	650.061	153831.8	0.8	5d 3D_1 485258.0 – 5f 1P_1 639089
4.2	29	719.360	139012.4	-0.4	5d 1P_1 474640.2 – 5f 3D_1 613653
0.4	24	722.089	138487.1	0.7	5d 3G_4 473554.6 – 5f 1F_3 612041
4.7	53	723.116	138290.5	1.4	5d 3G_3 484040.9 – 5f 3G_3 622330
10.2	67	724.671	137993.6	1.4	5d 3S_1 468443.8 – 5f 3P_2 606436
10.8	46	730.114	136964.9	0.5	5d 3G_4 473554.6 – 5f 1G_4 610519
10.6	71	732.926	136439.5	1.5	5d 3G_5 474397.0 – 5f 3G_5 610835
13.0	89	733.272	136375.0	-0.2	5d 3S_1 468443.8 – 5f 3P_1 604819
5.9	73	737.930	135514.3	0.1	5d 3S_1 468443.8 – 5f 3P_0 603958
6.3	49	738.231	135458.9	0.7	5d 1G_4 485906.8 – 5f 3G_4 621365
10.0	56	739.748	135181.3	1.5	5d 3D_2 487150.2 – 5f 3G_3 622330
18.3	98	740.770	134994.6	0.6	5d 3P_2 474361.0 – 5f 3D_3 609355
6.9	53	741.727	134820.5	-1.5	5d 3P_2 474361.0 – 5f 1D_2 609183
13.4	133	743.249	134544.5	1.7	5d 1P_1 474640.2 – 5f 1D_2 609183
7.6	83	743.435	134510.7	0.6	5d 1F_3 477530.9 – 5f 1F_3 612041
19.2	108	743.591	134482.5	-1.1	5d 3F_2 487846.4 – 5f 3G_3 622330
70.7	230	743.703	134462.2	-0.2	5d 3G_4 473554.6 – 5f 3H_5 608017
10.1	96	743.870	134432.1	-1.9	5d 3D_3 476085.0 – 5f 1G_4 610519
18.9	41	744.286	134356.9	0.3	5d 3P_1 482777.4 – 5f 3D_2 617134
19.4	172	744.962	134235.1	-0.3	5d 1D_2 477805.6 – 5f 1F_3 612041
20.5	143	745.282	134177.4	0.4	5d 3D_1 485258.0 – 5f 3F_2 619435
8.0	618b	745.627	134115.3	3.7	5d 3P_0 479541.4 – 5f 3D_1 613653 Sb V
56.8	191	746.843	133897.0	-0.1	5d 3G_3 484040.9 – 5f 3H_4 617938
25.4	89	747.172	133838.1	-0.9	5d 3D_3 476085.0 – 5f 3F_4 609924
2.9	31	748.386	133620.8	0.8	5d 3G_5 474397.0 – 5f 3H_5 608017
7.2	51	748.771	133552.1	0.4	5d 3F_3 488778.3 – 5f 3G_3 622330
21.5	136	750.293	133281.3	-0.5	5d 3D_2 487150.2 – 5f 3F_3 620432
20.3	120	750.360	133269.4	-0.6	5d 3D_3 476085.0 – 5f 3D_3 609355
69.0	252	751.541	133060.0	-0.2	5d 1G_4 485906.8 – 5f 1H_5 618967
36.0	157	751.939	132989.5	1.4	5d 1F_3 477530.9 – 5f 1G_4 610519
86.2	325	753.302	132748.9	-0.1	5d 3G_5 474397.0 – 5f 3H_6 607146
41.6	198	754.231	132585.3	-1.4	5d 3F_3 488778.3 – 5f 3G_4 621365
15.6				-0.3	5d 3F_2 487846.4 – 5f 3F_3 620432
54.7	216	754.413	132553.5	0.1	5d 3F_4 478281.6 – 5f 3G_5 610835
10.9	95	755.320	132394.2	1.1	5d 1F_3 477530.9 – 5f 3F_4 609924
12.8	53	757.156	132073.2	-1.8	5d 3P_2 474361.0 – 5f 3P_2 606436
3.9	15	758.292	131875.2	-0.8	5d 3D_1 485258.0 – 5f 3D_2 617134
17.9	66	759.630	131643.0	0.6	5d 3F_4 478281.6 – 5f 3F_4 609924
7.5	33	759.952	131587.3	-1.3	5d 3F_2 487846.4 – 5f 3F_2 619435
8.2	100m	761.160	131378.4	1.0	5d 1D_2 477805.6 – 5f 1D_2 609183 O V
5.5				-1.3	5d 1S_0 507709.3 – 5f 1P_1 639089
2.2	19	762.924	131074.7	1.3	5d 3F_4 478281.6 – 5f 3D_3 609355
3.0	21	764.087	130875.2	-0.4	5d 3P_1 482777.4 – 5f 3D_1 613653
6.4	55	766.534	130457.4	-0.6	5d 3P_2 474361.0 – 5f 3P_1 604819
2.6	18	767.157	130351.3	0.3	5d 3D_3 476085.0 – 5f 3P_2 606436
8.4	16	769.324	129984.2	0.4	5d 3D_2 487150.2 – 5f 3D_2 617134

gA values are in 10^9 s $^{-1}$ units.

a – arbitrary intensity units over a 1–1000 scale.

$\Delta\sigma$ = difference between the observed and the calculated (derived from the energy levels) values, in cm $^{-1}$.

b – blended line.

c – masked line.

Table II. Identified spectral lines in Te VII.

<i>gA</i>	<i>I(a)</i>	λ (Å)	σ (cm $^{-1}$)	$\Delta\sigma$	Transition		
<i>Resonance transitions</i>							
1505.0	233*	129.463	772421.5	-3.5	4d 1S_0	0.0 - 5f 1P_1	772425
51.2	194*	135.375	738688.8	-0.2	4d 1S_0	0.0 - 5f 3D_1	738689
<i>5p - 5d transitions (addition to [14])</i>							
14.6	176	542.582	184304.0	0.1	5p 1P_1	430409.1 - 5d 1S_0	614713.0
0.3	12	542.900	184196.1	-0.2	5p 3P_2	407633.1 - 5d 3F_3	591829.4
0.3	7	548.823	182208.2	-0.9	5p 3P_2	407633.1 - 5d 3D_2	589842.2
0.5	19	552.802	180896.5	2.0	5p 3F_3	410934.9 - 5d 3F_3	591829.4
1.3	76	565.120	176953.6	1.5	5p 3P_2	407633.1 - 5d 3P_1	584585.2
2.6	40	568.887	175781.8	-0.2	5p 3D_1	438931.0 - 5d 1S_0	614713.0
1.3	41	571.535	174967.3	-1.1	5p 3F_3	410934.9 - 5d 3G_3	585903.3
1.1	28	584.107	171201.5	-1.7	5p 3P_2	407633.1 - 5d 1D_2	578836.3
0.6	16	585.319	170847.0	-1.9	5p 3F_2	420980.5 - 5d 3F_3	591829.4
9.0	218	592.152	168875.6	-1.9	5p 3P_1	420964.7 - 5d 3D_2	589842.2
2.0	134	592.200	168861.8	0.1	5p 3F_2	420980.5 - 5d 3D_2	589842.2
0.6	22	593.230	168568.7	-1.8	5p 3F_3	410934.9 - 5d 3F_4	579505.4
3.4	127	595.591	167900.4	-1.0	5p 3F_3	410934.9 - 5d 1D_2	578836.3
1.2	50	601.963	166123.2	0.8	5p 3F_4	422311.9 - 5d 1G_4	588434.3
2.8	78	613.431	163017.5	1.6	5p 1D_2	427539.5 - 5d 3F_2	590555.4
1.4	61	615.977	162343.7	2.0	5p 3D_3	429487.7 - 5d 3F_3	591829.4
1.7	75	616.138	162301.3	-1.4	5p 1D_2	427539.5 - 5d 3D_2	589842.2
0.4	53	623.611	160356.4	1.9	5p 3D_3	429487.7 - 5d 3D_2	589842.2
0.4	56	639.315	156417.4	1.8	5p 3D_3	429487.7 - 5d 3G_3	585903.3
1.3	49	642.774	155575.6	1.7	5p 3F_2	420980.5 - 5d 3D_3	576554.4
1.2	37	669.568	149350.1	1.5	5p 3D_3	429487.7 - 5d 1D_2	578836.3
0.1	9	671.068	149016.1	1.2	5p 1D_2	427539.5 - 5d 3D_3	576554.4
0.5	17	680.063	147045.2	1.6	5p 1D_2	427539.5 - 5d 3P_2	574583.1
0.5	14	682.535	146512.6	-1.5	5p 3F_2	420980.5 - 5d 3S_1	567494.6
0.3	9	683.097	146392.1	-0.9	5p 3D_2	441069.6 - 5d 3D_1	587462.6
0.7	16	706.498	141543.2	1.3	5p 1F_3	436847.2 - 5d 1F_3	578389.1
<i>5d - 5f transitions</i>							
0.5	51	595.159	168022.3	-1.3	5d 3F_4	579505.4 - 5f 1G_4	747529
9.5	359b	610.847	163707.0	-3.8	5d 1P_1	574978.2 - 5f 3D_1	738689 O III
19.8	620b	614.188	162816.6	0.2	5d 3S_1	567494.6 - 5f 3P_2	730311 Te V
10.4	12	615.344	162510.7	2.0	5d 3G_3	585903.3 - 5f 3G_3	748412
21.5	36	619.925	161309.8	0.8	5d 3G_4	573537.0 - 5f 1G_4	734846
25.0	60	621.024	161024.4	1.0	5d 3S_1	567494.6 - 5f 3P_1	728518
3.4	7	621.401	160926.7	0.9	5d 3P_1	584585.2 - 5f 3F_2	745511
20.3	42	622.485	160646.4	1.7	5d 3G_5	574747.3 - 5f 3G_5	735392
11.2	35	625.672	159828.2	0.8	5d 3S_1	567494.6 - 5f 3P_0	727322
0.5	7	626.539	159607.0	-0.7	5d 3G_3	585903.3 - 5f 3F_2	745511
7.3	28	628.556	159094.8	0.1	5d 1G_4	588434.3 - 5f 3G_4	747529
37.9	72	629.209	158929.7	0.8	5d 3P_2	574583.1 - 5f 3D_3	733512
14.6	29	630.097	158705.7	-1.2	5d 3P_2	574583.1 - 5f 1D_2	733290
25.6	88	630.635	158570.2	0.4	5d 3D_2	589842.2 - 5f 3G_3	748412
137.2	186	631.349	158390.9	-0.1	5d 3G_4	573537.0 - 5f 3H_5	731928
27.5	47	631.663	158312.3	0.5	5d 1P_1	574978.2 - 5f 1D_2	733290
21.2	37	631.740	158293.1	1.5	5d 3D_3	576554.4 - 5f 1G_4	734846
32.9	93	632.315	158148.9	-1.9	5d 3P_1	584585.2 - 5f 3D_2	742736
22.8	55	632.533	158094.6	0.7	5d 1F_3	578389.1 - 5f 1F_3	736483
39.7	82	632.719	158048.0	-0.4	5d 3D_1	587462.6 - 5f 3F_2	745511
35.3	191b	633.485	157856.9	0.3	5d 3F_2	590555.4 - 5f 3G_3	748412 DI [14]
16.3	31	633.668	157811.4	0.4	5d 3P_0	580878.0 - 5f 3D_1	738689
10.5	64	634.067	157712.1	0.1	5d $1S_0$	614713.0 - 5f 1P_1	772425
58.3	87	634.330	157646.8	0.1	5d 1D_2	578836.3 - 5f 1F_3	736483
110.9	169	634.411	157626.6	-0.1	5d 3G_3	585903.3 - 5f 3H_4	743530
49.6	85	634.782	157534.3	1.7	5d 3D_3	576554.4 - 5f 3F_4	734087
41.3	55	637.122	156955.8	-1.8	5d 3D_3	576554.4 - 5f 3D_3	733512
36.6	35	637.614	156834.8	0.0	5d 3D_2	589842.2 - 5f 3F_3	746677
4.4	10	638.010	156737.3	1.7	5d 3D_3	576554.4 - 5f 1D_2	733290
14.2	160b	638.656	156578.8	-3.8	5d 3F_3	591829.4 - 5f 3G_3	748412
70.2	104	639.157	156456.0	-0.9	5d 1F_3	578389.1 - 5f 1G_4	734846
164.9	279	639.555	156358.7	0.0	5d 3G_5	574747.3 - 5f 3H_6	731106
135.7	186	639.805	156297.7	0.0	5d 3G_4	588434.3 - 5f 1H_5	744732
37.4	84	640.526	156121.6	0.0	5d 3F_2	590555.4 - 5f 3F_3	746677
103.8	213	641.499	155884.9	-1.7	5d 3F_4	579505.4 - 5f 3G_5	735392
23.4	64	642.151	155726.6	-1.3	5d 3P_2	574583.1 - 5f 3P_2	730311
47.4	165	642.261	155700.0	0.4	5d 3F_3	591829.4 - 5f 3G_4	747529

Table II. *Continued.*

<i>gA</i>	<i>I(a)</i>	λ (Å)	σ (cm ⁻¹)	$\Delta\sigma$	Transition	
21.3				2.1	5d ¹ F ₃	578389.1 – 5f ³ F ₄ 734087
5.5	19	642.389	155669.0	0.2	5d ³ D ₂	589842.2 – 5f ³ F ₂ 745511
5.4	22	643.785	155331.5	-1.3	5d ¹ P ₁	574978.2 – 5f ³ P ₂ 730311
8.6	34	644.031	155272.1	-1.3	5d ³ D ₁	587462.6 – 5f ³ D ₂ 742736
13.1	42	645.348	154955.1	-0.5	5d ³ F ₂	590555.4 – 5f ³ F ₂ 745511
35.2	134	646.914	154580.2	-1.4	5d ³ F ₄	579505.4 – 5f ³ F ₄ 734087
15.6	32	647.435	154455.6	1.9	5d ¹ D ₂	578836.3 – 5f ¹ D ₂ 733290
6.2	13	648.913	154103.9	0.1	5d ³ P ₁	584585.2 – 5f ³ D ₁ 738689
11.8	26	649.629	153934.0	-0.9	5d ³ P ₂	574583.1 – 5f ³ P ₁ 728518
15.0	39	654.042	152895.4	1.6	5d ³ D ₂	589842.2 – 5f ³ D ₂ 742736
9.0	66	660.171	151475.9	1.2	5d ¹ D ₂	578836.3 – 5f ³ P ₂ 730311
0.6	523b	700.599	142735.0	-1.8	5d ³ P ₁	584585.2 – 5f ³ P ₀ 727322
0.1	19	715.010	139858.1	-1.3	5d ³ D ₁	587462.6 – 5f ³ P ₀ 727322

* – these lines have been identified earlier (see text). See also the footnotes to Table I.

figurations and the odd 4d⁹np ($n = 5, 6$), 4d⁹nf ($n = 4–6$), 4d⁸5s5p, 4d⁸5p5d, 4p⁵4d¹⁰5s and 4p⁵4d¹⁰5d configurations. For the unknown configurations we scaled the Slater energy parameters to 0.85 of their *ab initio* Hartree–Fock values.

Accurate *ab initio* prediction of the 4d⁹5d ¹S₀ energies is difficult because they depend on the Slater integral $G^0(4d, 5d)$ and on various configuration interactions. We followed the same approach as it was done for Ni-like ions in which the 3d⁹4p ¹P₁ – 3d⁹4d ¹S₀ transitions were surveyed by MCDF calculations and corrected for systematic $E_{\text{exp}} - E_{\text{MCDF}}$ deviations [20]. In the Pd I isoelectronic sequence, considering the laser effect on the 4d⁹5p ¹P₁ – 4d⁹5d ¹S₀ transition in Xe IX ($\lambda = 418.1$ Å) [1] as a proof of the correctness of its identification and using the Ag II data [2], we interpolated the known differences between experimental and theoretical wavenumbers of this transition to the other ions.

3. Results and discussion

The preliminary analysis of the obtained spectrograms showed that the spectral lines of Pd-like ions are intense in the “hot” vacuum spark spectra and become weaker or completely absent in the “cold” sliding spark ones. The clear ionization character of the lines was helpful in the present analysis for choosing the lines belonging to a particular spectrum.

The results of our line identifications are presented in Tables I, II and III respectively for Sb VI, Te VII and I VIII.

We completely confirm the previous analyses of the 4d⁹s – 4d⁹5p and 4d⁹5p – 4d⁹5d transitions in Sb VI and Te VII [7,14] and of the 4d⁹5p – 4d⁹6s transitions in Sb VI [14], our wavelengths and level energies being in good agreement with the previously published data. Therefore only the additional wavelengths are reported here, namely six previously unknown relatively weak lines of the 4d⁹5p – 4d⁹(5d + 6s) transitions in Sb VI and twenty-six of the 4d⁹5p – 4d⁹5d transitions in Te VII. In both spectra, the 4d⁹5d ¹S₀ levels were found from respectively three and two transitions to 4d⁹5p levels. Moreover, we newly classified lines corresponding to the 4d⁹5d – 4d⁹5f transitions in Sb VI and Te VII including the 4d⁹5d ¹S₀ – 4d⁹5f ¹P₁ transitions in both spectra.

For I VIII, out of the twenty-five 4d⁹5s – 4d⁹5p transitions given in Table III, eighteen were correctly identified in [8]. However our wavelengths show systematic red shifts of about 0.01–0.03 Å against the wavelengths measured in [8]. The resulting revised 4d⁹5s and 4d⁹5p level energies are 10–50 cm⁻¹ lower than the previous values. On the basis of the new 4d⁹5p energies we identified the 4d⁹5p – 4d⁹5d transition array and determined the energies of all the 4d⁹5d levels in I VIII, including the ¹S₀ level. All the forty-six 4d⁹5p 4d⁹5d lines given in Table III are new, the 4d⁹5d ¹S₀ and 4d⁹5d ³G₅ levels being derived each from one single transition. The improved energy values of 4d⁹5p $J = 1$ levels derived from the new measurements are supported by numerous 4d⁹5s – 4d⁹5p and 4d⁹5p – 4d⁹5d transitions. Unfortunately we could not identify unambiguously any 4d⁹5d – 4d⁹5f transition in I VIII, not even the most intense ones. The probable reason is that the source temperature was not high enough to excite a well-developed spectrum of the transitions between high lying configurations.

All the experimentally determined level energies in Sb VI, Te VII and I VIII are respectively given in Tables IV, V and VI, together with the fitted energies and the corresponding wavefunction compositions from the parametric study of the configurations. For the level designations in Tables I–III we used the first *LS*-terms in the level wavefunction compositions given in Tables IV–VI. It should be noted that, for some levels, these first terms do not coincide with the largest percentage terms. It is seen from Tables IV–VI that the *Jj* coupling scheme would be more appropriate than the *LS* coupling scheme for the level designation, but the *LS* labels are used for the sake of consistency with previous papers. The energies of the lower and upper levels are also given for the transitions in Tables I–III.

It is seen from the Tables that all the measured wavenumbers agree with the level energy differences within the accuracy of the averaged level energies (1–2 cm⁻¹). The new resonance wavenumbers agree with the 5–5 transition arrays within an accuracy better than ± 10 cm⁻¹. The measured line intensities are in good agreement with the calculated *gA* values of the corresponding transitions. The structures of the investigated configurations are described quite well by the least squared fits (LSF) of energy parameters. Moreover, the deviations of the experimental energies from the fitted ones for the separate levels vary monotonously along the isoelectronic sequence.

Table III. Identified spectral lines in VIII.

<i>gA</i>	<i>I(a)</i>	λ (Å)	σ (cm $^{-1}$)	$\Delta\sigma$	Transition
<i>Resonance transitions</i>					
1803.0	130*	110.479	905147.8	-0.3	4d 1S_0 0 - 5f 1P_1 905148
49.5	50*	115.079	868968.3	1.3	4d 1S_0 0 - 5f 3D_1 868967
33.4	850*	190.152	525895.1	0.1	4d 1S_0 0 - 5p 3D_1 525895
191.3	950*	194.155	515052.4	-5.6	4d 1S_0 0 - 5p 1P_1 515058
0.9	120*	197.947	505185.7	-8.3	4d 1S_0 0 - 5p 3P_1 505194
<i>5p - 5d transitions</i>					
20.9	32	472.262	211746.9	-0.1	5p 1P_1 515058 - 5d 1S_0 726805
2.6	72	515.606	193946.4	-0.6	5p 3F_2 504541 - 5d 3F_2 698488
2.0	22	517.575	193208.6	-0.4	5p 3F_2 504541 - 5d 3D_2 697750
37.1	167	518.353	192918.6	0.6	5p 3P_2 489118 - 5d 3D_3 682036
10.4	55	519.327	192556.8	0.8	5p 3P_1 505194 - 5d 3D_2 697750
4.3	17	519.812	192377.2	1.2	5p 3F_3 492554 - 5d 1D_2 684930
18.1	181	521.435	191778.5	1.5	5p 3F_3 492554 - 5d 1F_3 684331
9.2	36	522.800	191277.7	0.7	5p 3P_2 489118 - 5d 1P_1 680395
55.7	174	524.380	190701.3	1.3	5p 3P_2 489118 - 5d 3P_2 679818
33.0	148	527.756	189481.7	-0.3	5p 3F_3 492554 - 5d 3D_3 682036
73.0	307	530.691	188433.7	-1.3	5p 3F_2 504541 - 5d 3G_3 692976
8.3	54	534.003	187265.0	1.0	5p 3F_3 492554 - 5d 3P_2 679818
11.4	55	536.400	186428.1	0.1	5p 3P_1 505194 - 5d 3P_1 691622
134.0	403	537.673	185986.7	-0.3	5p 3F_3 492554 - 5d 3G_4 678541
17.3	55	545.164	183431.0	1.0	5p 1P_1 515058 - 5d 3F_2 698488
5.8	16	547.367	182692.7	0.7	5p 1P_1 515058 - 5d 3D_2 697750
35.5	198	547.919	182508.6	0.6	5p 3P_2 489118 - 5d 3S_1 671626
14.9	97	548.943	182168.2	0.2	5p 3P_1 505194 - 5d 3P_0 687362
30.5	118	553.916	180532.6	-1.4	5p 1D_2 512442 - 5d 3G_3 692976
7.3	25	554.363	180387.1	-1.9	5p 3F_2 504541 - 5d 1D_2 684930
25.3	108	556.206	179789.5	-0.5	5p 3F_2 504541 - 5d 1F_3 684331
15.9	85	556.371	179736.1	0.1	5p 3P_1 505194 - 5d 1D_2 684930
17.7	166	558.922	178915.8	-0.2	5p 3P_0 516034 - 5d 3D_1 694950
38.5	254	559.305	178793.3	0.3	5p 3F_4 506971 - 5d 3F_4 685764
9.4	44	566.368	176563.6	-0.4	5p 1P_1 515058 - 5d 3P_1 691622
23.9	102	567.078	176342.7	1.7	5p 1F_3 523790 - 5d 3F_3 700131
12.7	77	570.773	175200.8	-0.2	5p 3P_1 505194 - 5d 1P_1 680395
7.6	54	571.216	175065.3	0.3	5p 3F_4 506971 - 5d 3D_3 682036
152.8	382	577.250	173235.1	0.1	5p 3F_4 506971 - 5d 3G_5 680206
29.6	118	579.397	172593.1	0.1	5p 3D_1 525895 - 5d 3F_2 698488
30.9	155	579.752	172487.6	-0.4	5p 1D_2 512442 - 5d 1D_2 684930
122.4	311	579.879	172449.8	-0.2	5p 1F_3 523790 - 5d 1G_4 696240
40.4	292	581.775	171887.9	-1.1	5p 1D_2 512442 - 5d 1F_3 684331
16.8	75	581.881	171856.4	1.4	5p 3D_1 525895 - 5d 3D_2 697750
69.2	232	582.305	171731.3	-0.8	5p 3D_2 528399 - 5d 3F_3 700131
8.2	45	582.849	171571.1	1.1	5p 3F_4 506971 - 5d 3G_4 678541
29.7	258	585.097	170911.8	-0.2	5p 3D_3 514852 - 5d 3F_4 685764
8.0	61	588.676	169872.7	0.7	5p 1P_1 515058 - 5d 1D_2 684930
15.7	119	590.039	169480.2	1.2	5p 3D_3 514852 - 5d 1F_3 684331
29.5	96	590.495	169349.5	-1.5	5p 3D_2 528399 - 5d 3D_2 697750
6.1	43	591.062	169187.0	1.0	5p 1F_3 523790 - 5d 3G_3 692976
29.7	98	598.146	167183.3	-0.7	5p 3D_3 514852 - 5d 3D_3 682036
4.0	20	600.850	166430.9	-1.1	5p 3P_1 505194 - 5d 3S_1 671626
11.1	62	604.828	165336.3	-0.7	5p 1P_1 515058 - 5d 1P_1 680395
13.2	46	606.190	164964.9	-1.1	5p 3D_3 514852 - 5d 3P_2 679818
6.2	28	610.922	163687.1	-1.9	5p 3D_3 514852 - 5d 3G_4 678541
2.1	38	628.210	159182.4	-1.6	5p 1D_2 512442 - 5d 3S_1 671626
<i>5s - 5p transitions</i>					
1.4	58	693.067	144286.2	-0.8	5s 3D_2 381608 - 5p 3D_1 525895
1.9	117	703.316	142183.6	1.6	5s 3D_2 381608 - 5p 1F_3 523790
20.5	370*	732.642	136492.3	0.3	5s 3D_3 378360 - 5p 3D_3 514852
7.8	187*	736.545	135769.0	-1.0	5s 3D_1 392629 - 5p 3D_2 528399
0.8	30	745.805	134083.3	1.3	5s 3D_3 378360 - 5p 1D_2 512442
2.9	114*	749.338	133451.1	1.1	5s 3D_2 381608 - 5p 1P_1 515058
10.7	185*	750.380	133265.8	-0.3	5s 3D_1 392629 - 5p 3D_1 525895
8.5	215*	750.502	133244.2	0.2	5s 3D_2 381608 - 5p 3D_3 514852
12.9	225*	755.234	132409.3	0.3	5s 1D_2 395990 - 5p 3D_2 528399
14.5	272*	764.332	130833.3	-0.8	5s 3D_2 381608 - 5p 1D_2 512442
0.9	10	769.791	129905.3	0.3	5s 1D_2 395990 - 5p 3D_1 525895
34.7	364*	777.537	128611.3	0.3	5s 3D_3 378360 - 5p 3F_4 506971
24.5	278*	782.476	127799.5	-0.5	5s 1D_2 395990 - 5p 1F_3 523790

Table III. *Continued.*

<i>gA</i>	<i>I(a)</i>	λ (Å)	σ (cm $^{-1}$)	$\Delta\sigma$	Transition
6.8	202	809.146	123587.1	1.1	5s 3D_2 381608 – 5p 3P_1 505194
3.3	71*	810.341	123404.9	-0.1	5s 3D_1 392629 – 5p 3P_0 516034
4.4	97*	813.450	122933.1	0.1	5s 3D_2 381608 – 5p 3F_2 504541
5.8	77*	839.862	119067.2	-0.8	5s 1D_2 395990 – 5p 1P_1 515058
1.4	41	841.316	118861.4	-0.6	5s 1D_2 395990 – 5p 3D_3 514852
2.2	51*	858.721	116452.3	0.3	5s 1D_2 395990 – 5p 1D_2 512442
6.3	160*	875.701	114194.2	0.2	5s 3D_3 378360 – 5p 3F_3 492554
6.9	165*	893.562	111911.6	-0.4	5s 3D_1 392629 – 5p 3F_2 504541
11.8	190*	901.342	110945.7	-0.3	5s 3D_2 381608 – 5p 3F_3 492554
11.8	211*	902.864	110758.7	0.7	5s 3D_3 378360 – 5p 3P_2 489118
2.1	32	915.719	109203.8	-0.2	5s 1D_2 395990 – 5p 3P_1 505194
2.6	36*	921.220	108551.7	0.7	5s 1D_2 395990 – 5p 3F_2 504541

See the footnotes to Tables I and II.

The LSF and the *ab initio* Hartree–Fock (HF) energy parameters of the studied configurations are presented in Table VII. The average LSF parameter deviations of the fits are given in brackets. All the configuration interaction parameters were fixed at 0.85 of their HF values.

Although the 4d⁹5d 1S_0 level energy in I VIII has been determined only by one single line at 472.262 Å (Table III), its value is secured by the absence of any other suitable line in the corresponding region of the iodine spectrum. Moreover, the experimental energies of this level so as the LSF/HF G^0 (4d, 5d) parameter ratios (see Table VII) have very monotonous behaviour along the isoelectronic sequence. On the basis of our results the wavelengths of the laser transition 4d⁹5p 1P_1 – 4d⁹5d 1S_0 can be predicted for Cs X, Ba XI and La XII ions respectively at 375.25 ± 0.20 Å, 340.3 ± 0.3 Å and 311.4 ± 0.5 Å.

Unfortunately we could not identify the other transition of laser interest, 4d⁹5d 1P_1 – 4d⁹5f 1P_1 [1], because it is too weak in the studied ions. According to *ab initio* calculations, the 4d⁹5d 1S_0 – 4d⁹5f 1P_1 transition is more intense for the relatively light Pd-like ions through Xe IX, and has been identified by us in Sb VI and Te VII ions (see Tables I and II).

Furthermore, the present step in the analysis of Pd-like ion spectra did not improve our knowledge of the 4d⁹4f configurations. Extended observations in higher charged ions where 4d⁹4f is the lowest odd parity configuration [11] will be necessary. Systematic parametric studies of 4d^{*n*}4f^{*m*} configurations in known spectra are in progress following Cowan's method [19] in order to predict all relevant energy parameters of 4d⁹4f with the best accuracy.

Table IV. The level energies for Sb VI (cm $^{-1}$).

<i>E(exp)</i>	<i>E(fit)</i>	ΔE	LS-coupling terms	<i>Jj</i> -coupling terms
Even configurations:				
<i>J</i> = 0				
0.0	0	0	100% 4d 1S	100% 4d (3/2,3/2)
479541.4b	479496	45	97% 5d 3P + 2% 5d 1S	55% 5d (5/2,5/2)
507709.3	507710	-1	94% 5d 1S + 4% 6d 1S	53% 5d (3/2,3/2)
<i>J</i> = 1				
253230.6a	253219	11	100% 5s 3D	100% 5s (3/2,1/2)
468443.8b	468496	-52	82% 5d 3S + 15% 5d 3P	61% 5d (5/2,3/2)
474640.2b	474742	-102	51% 5d 1P + 25% 5d 3D	64% 5d (5/2,5/2)
482777.4b	482826	-48	41% 5d 3P + 40% 5d 1P	53% 5d (3/2,5/2)
485258.0b	485222	36	71% 5d 3D + 21% 5d 3P	58% 5d (3/2,3/2)
525023.2b	525020	3	100% 6s 3D	100% 6s (3/2,1/2)
<i>J</i> = 2				
245663.8a	245633	31	68% 5s 3D + 32% 5s 1D	92% 5s (5/2,1/2)
256382.2a	256397	-15	68% 5s 1D + 32% 5s 3D	92% 5s (3/2,1/2)
474361.0b	474351	10	61% 5d 3P + 36% 5d 3D	77% 5d (5/2,3/2)
477805.6b	477820	-15	46% 5d 1D + 20% 5d 3D	75% 5d (5/2,5/2)
487150.2b	487145	5	38% 5d 3D + 41% 5d 1D	83% 5d (3/2,5/2)
487846.4b	487882	-36	81% 5d 3F + 12% 5d 1D	85% 5d (3/2,3/2)
515506.6b	515504	3	53% 6s 1D + 47% 6s 3D	99% 6s (5/2,1/2)
525662.0b	525665	-3	53% 6s 3D + 47% 6s 1D	99% 6s (3/2,1/2)
<i>J</i> = 3				
242916.8a	242944	-28	100% 5s 3D	100% 5s (5/2,1/2)
476085.0b	476048	37	63% 5d 3D + 29% 5d 3F	73% 5d (5/2,3/2)
477530.9b	477530	1	44% 5d 1F + 24% 5d 3D	72% 5d (5/2,5/2)
484040.9b	483998	42	73% 5d 3G + 19% 5d 1F	90% 5d (3/2,3/2)
488778.3b	488840	-61	50% 5d 3F + 35% 5d 1F	94% 5d (3/2,5/2)

Table IV. *Continued.*

<i>E(exp)</i>	<i>E(fit)</i>	ΔE	<i>LS</i> -coupling terms	<i>Jj</i> -coupling terms
514662.0b <i>J</i> = 4	514665	−3	100% 6s ^3D	100% 6s (5/2,1/2)
473554.6b	473544	11	55% 5d ^3G + 43% 5d ^1G	96% 5d (5/2,3/2)
478281.6b	478297	−16	77% 5d ^3F + 18% 5d ^1G	94% 5d (5/2,5/2)
485906.8b <i>J</i> = 5	485861	46	39% 5d ^1G + 40% 5d ^3G	97% 5d (3/2,5/2)
474397.0b	474300	97	100% 5d ^3G	100% 5d (5/2,5/2)
Odd configurations:				
<i>J</i> = 0				
349101.6a	349038	63	100% 5p ^3P	100% 5p (3/2,3/2)
603958	603940	18	99% 5f ^3P + 1% 4f ^3P	99% 5f (5/2,5/2)
<i>J</i> = 1				
341970.6a	341944	27	86% 5p ^3P + 13% 5p ^3D	47% 5p (5/2,3/2)
351009.3a	351025	−16	80% 5p ^1P + 19% 5p ^3D	62% 5p (3/2,1/2)
357446.0a	357440	6	67% 5p ^3D + 19% 5p ^1P	81% 5p (3/2,3/2)
604819	604972	−153	88% 5f ^3P + 11% 5f ^3D	80% 5f (5/2,5/2)
613653	613739	−86	86% 5f ^3D + 10% 5f ^3P	35% 5f (5/2,7/2)
639089	639088	1	54% 5f ^1P + 28% 6f ^1P	33% 5f (3/2,5/2)
<i>J</i> = 2				
331122.8a	331187	−64	82% 5p ^3P + 13% 5p ^3D	86% 5p (5/2,1/2)
342575.0a	342592	−17	87% 5p ^3F + 8% 5p ^3D	81% 5p (3/2,1/2)
347920.1a	347987	−67	67% 5p ^1D + 20% 5p ^3D	72% 5p (5/2,3/2)
359232.1a	359240	−8	59% 5p ^3D + 30% 5p ^1D	95% 5p (3/2,3/2)
606436	606464	−28	62% 5f ^3P + 22% 5f ^3D	69% 5f (5/2,7/2)
609183	609182	1	37% 5f ^1D + 38% 5f ^3F	75% 5f (5/2,5/2)
617134	616995	139	37% 5f ^3D + 35% 5f ^3P	84% 5f (3/2,7/2)
619435	619486	−51	61% 5f ^3F + 22% 5f ^1D	90% 5f (3/2,5/2)
<i>J</i> = 3				
334262.5a	334173	89	56% 5p ^3F + 33% 5p ^1F	97% 5p (5/2,1/2)
349411.7a	349304	108	72% 5p ^3D + 28% 5p ^1F	97% 5p (5/2,3/2)
355419.9a	355461	−41	39% 5p ^1F + 44% 5p ^3F	97% 5p (3/2,3/2)
609355	609422	−67	33% 5f ^3D + 29% 5f ^3F	40% 5f (5/2,5/2)
612041	612079	−38	37% 5f ^1F + 20% 5f ^3G	54% 5f (5/2,7/2)
620432	620449	−17	38% 5f ^3F + 32% 5f ^3G	86% 5f (3/2,7/2)
622330	622364	−34	40% 5f ^3G + 49% 5f ^1F	84% 5f (3/2,5/2)
<i>J</i> = 4				
342977.0a	343057	−80	100% 5p ^3F	100% 5p (5/2,3/2)
609924	609835	89	80% 5f ^3F + 13% 5f ^3G	81% 5f (5/2,7/2)
610519	610506	13	42% 5f ^1G + 30% 5f ^3G	79% 5f (5/2,5/2)
617938	617979	−41	72% 5f ^3H + 15% 5f ^1G	90% 5f (3/2,5/2)
621365	621363	2	33% 5f ^3G + 29% 5f ^1G	73% 5f (3/2,7/2)
<i>J</i> = 5				
608017	607898	119	60% 5f ^3H + 38% 5f ^1H	98% 5f (5/2,5/2)
610835	610868	−33	76% 5f ^3G + 18% 5f ^1H	97% 5f (5/2,7/2)
618967	618913	54	43% 5f ^1H + 35% 5f ^3H	97% 5f (3/2,7/2)
<i>J</i> = 6				
607146	607067	79	100% 5f ^3H	100% 5f (5/2,7/2)

a – energy value taken from [7].

b – energy value taken from [14]. Note that the two $J = 2$ levels at 515506.6 and 525662.0 cm^{-1} have their *LS* designations exchanged compared with [14]. $\Delta E = E(\text{exp}) - E(\text{fit})$.Table V. *The level energies for Te VII (cm^{−1}).*

<i>E(exp)</i>	<i>E(fit)</i>	ΔE	<i>LS</i> -coupling terms	<i>Jj</i> -coupling terms
Even configurations:				
<i>J</i> = 0				
0.0	0	0	100% 4d ^1S	100% 4d (3/2,3/2)
580878.0b	580806	72	98% 5d ^3P + 2% 5d ^1S	54% 5d (5/2,5/2)
614713.0	614715	−2	95% 5d ^1S + 3% 6d ^1S	53% 5d (3/2,3/2)
<i>J</i> = 1				
320311.6a	320298	14	100% 5s ^3D	100% 5s (3/2,1/2)
567494.6b	567549	−54	82% 5d ^3S + 16% 5d ^3P	62% 5d (5/2,3/2)
574978.2b	575125	−147	51% 5d ^1P + 25% 5d ^3D	65% 5d (5/2,5/2)
584585.2b	584656	−71	38% 5d ^3P + 42% 5d ^1P	47% 5d (3/2,5/2)

Table V. *Continued.*

<i>E(exp)</i>	<i>E(fit)</i>	ΔE	<i>LS</i> -coupling terms	<i>Jj</i> -coupling terms
587462.6b	587413	50	69% 5d 3D + 24% 5d 3P	52% 5d ($3/2,3/2$)
647795.2b	647790	5	100% 6s 3D	100% 6s ($3/2,1/2$)
<i>J</i> = 2				
311123.3a	311091	32	65% 5s 3D + 35% 5s 1D	94% 5s ($5/2,1/2$)
323571.2a	323588	-17	65% 5s 1D + 35% 5s 3D	94% 5s ($3/2,1/2$)
574583.1b	574569	14	59% 5d 3P + 38% 5d 3D	80% 5d ($5/2,3/2$)
578836.3b	578860	-24	45% 5d 1D + 22% 5d 3P	78% 5d ($5/2,5/2$)
589842.2b	589852	-10	35% 5d 3D + 46% 5d 1D	75% 5d ($3/2,5/2$)
590555.4b	590591	-35	82% 5d 3F + 9% 5d 3D	78% 5d ($3/2,3/2$)
636483.1b	636479	4	53% 6s 1D + 47% 6s 3D	99% 6s ($5/2,1/2$)
648496.0b	648501	-5	53% 6s 3D + 47% 6s 1D	100% 6s ($3/2,1/2$)
<i>J</i> = 3				
308119.2a	308148	-29	100% 5s 3D	100% 5s ($5/2,1/2$)
576554.4b	576528	27	60% 5d 3D + 31% 5d 3F	76% 5d ($5/2,3/2$)
578389.1b	578398	-9	42% 5d 1F + 27% 5d 3D	75% 5d ($5/2,5/2$)
585903.3b	585867	37	72% 5d 3G + 20% 5d 1F	90% 5d ($3/2,3/2$)
591829.4b	591890	-60	51% 5d 3F + 35% 5d 1F	95% 5d ($3/2,5/2$)
635542.2b	635547	-4	100% 6s 3D	100% 6s ($5/2,1/2$)
<i>J</i> = 4				
573577.0b	573542	35	56% 5d 3G + 42% 5d 1G	97% 5d ($5/2,3/2$)
579505.4b	579504	1	77% 5d 3F + 19% 5d 1G	95% 5d ($5/2,5/2$)
588434.3b	588373	61	39% 5d 1G + 40% 5d 3G	97% 5d ($3/2,5/2$)
<i>J</i> = 5				
574747.3b	574633	114	100% 5d 3G	100% 5d ($5/2,5/2$)
Odd configurations:				
<i>J</i> = 0				
429850.3a	429791	59	100% 5p 3P	100% 5p ($3/2,3/2$)
727322	727347	-25	100% 5f 3P	99% 5f ($5/2,5/2$)
<i>J</i> = 1				
420964.7a	420929	36	83% 5p 3P + 16% 5p 3D	44% 5p ($5/2,3/2$)
430409.1a	430428	-19	81% 5p 1P + 17% 5p 3D	57% 5p ($3/2,1/2$)
438931.0a	438927	4	67% 5p 3D + 18% 5p 1P	83% 5p ($3/2,3/2$)
728518	728547	-29	88% 5f 3P + 11% 5f 3D	80% 5f ($5/2,5/2$)
738689	738753	-64	87% 5f 3D + 11% 5f 3P	36% 5f ($5/2,7/2$)
772425	772424	1	62% 5f 1P + 19% 6f 1P	36% 5f ($3/2,5/2$)
<i>J</i> = 2				
407633.1a	407716	-83	80% 5p 3P + 15% 5p 3D	88% 5p ($5/2,1/2$)
420980.5a	420999	-19	87% 5p 3F + 7% 5p 3D	84% 5p ($3/2,1/2$)
427539.5a	427620	-81	66% 5p 1D + 20% 5p 3D	76% 5p ($5/2,3/2$)
441069.6a	441085	-15	58% 5p 3D + 29% 5p 1D	96% 5p ($3/2,3/2$)
730311	730338	-27	64% 5f 3P + 23% 5f 3D	70% 5f ($5/2,7/2$)
733290	733352	-62	38% 5f 1D + 39% 5f 3F	74% 5f ($5/2,5/2$)
742736	742646	90	29% 5f 3D + 29% 5f 3P	68% 5f ($3/2,7/2$)
745511	745416	95	61% 5f 3F + 22% 5f 1D	90% 5f ($3/2,5/2$)
<i>J</i> = 3				
410934.9a	410829	106	55% 5p 3F + 33% 5p 1F	98% 5p ($5/2,1/2$)
429487.6a	429371	117	72% 5p 3D + 27% 5p 1F	97% 5p ($5/2,3/2$)
436847.2a	436878	-31	39% 5p 1F + 45% 5p 3F	98% 5p ($3/2,3/2$)
733512	733527	-15	49% 5f 3D + 47% 5f 3F	63% 5f ($5/2,5/2$)
736483	736441	42	43% 5f 1F + 21% 5f 3G	61% 5f ($5/2,7/2$)
746677	746538	139	39% 5f 3F + 29% 5f 3G	89% 5f ($3/2,7/2$)
748412	748507	-95	45% 5f 3G + 47% 5f 1F	90% 5f ($3/2,5/2$)
<i>J</i> = 4				
422311.9a	422386	-74	100% 5p 3F	100% 5p ($5/2,3/2$)
734087	734141	-54	80% 5f 3F + 15% 5f 3G	79% 5f ($5/2,7/2$)
734846	734846	0	44% 5f 1G + 28% 5f 3G	76% 5f ($5/2,5/2$)
743530	743704	-174	74% 5f 3H + 15% 5f 1G	92% 5f ($3/2,5/2$)
747529	747502	27	38% 5f 3G + 30% 5f 1G	80% 5f ($3/2,7/2$)
<i>J</i> = 5				
731928	731816	112	59% 5f 3H + 40% 5f 1H	98% 5f ($5/2,5/2$)
735392	735416	-24	71% 5f 3G + 17% 5f 1H	90% 5f ($5/2,7/2$)
744732	744767	-35	42% 5f 1H + 36% 5f 3H	98% 5f ($3/2,7/2$)
<i>J</i> = 6				
731106	730990	116	100% 5f 3H	100% 5f ($5/2,7/2$)

See the footnotes to Table IV.

Table VI. The level energies for I VIII (cm^{-1}).

$E(\text{exp})$	$E(\text{fit})$	ΔE	LS-coupling terms	Jj-coupling terms
Even Configurations:				
$J = 0$				
0	0	0	100% 4d ^1S	100% 4d (3/2,3/2)
687273?	687221	52	98% 5d ^3P + 2% 5d ^1S	54% 5d (5/2,5/2)
726805	726806	-1	95% 5d ^1S + 2% 6d ^1S	53% 5d (3/2,3/2)
$J = 1$				
392629a	392613	16	100% 5s ^3D	100% 5s (3/2,1/2)
671626	671690	-64	82% 5d ^3S + 16% 5d ^3P	64% 5d (5/2,3/2)
680395	680556	-161	51% 5d ^1P + 25% 5d ^3D	67% 5d (5/2,5/2)
691622	691698	-76	34% 5d ^3P + 44% 5d ^1P	51% 5d (3/2,3/2)
694950	694874	76	66% 5d ^3D + 28% 5d ^3P	52% 5d (3/2,5/2)
-	777213	-	100% 6s ^3D	100% 6s (3/2,1/2)
$J = 2$				
381608a	381577	31	63% 5s ^3D + 37% 5s ^1D	95% 5s (5/2,1/2)
395990a	396008	-18	63% 5s ^1D + 37% 5s ^3D	95% 5s (3/2,1/2)
679818	679770	48	56% 5d ^3P + 40% 5d ^3D	83% 5d (5/2,3/2)
684930	684942	-12	45% 5d ^1D + 24% 5d ^3P	80% 5d (5/2,5/2)
697750	697772	-22	28% 5d ^3D + 51% 5d ^1D	60% 5d (3/2,5/2)
698488	698518	-30	80% 5d ^3F + 16% 5d ^3D	63% 5d (3/2,3/2)
-	763907	-	54% 6s ^1D + 46% 6s ^3D	100% 6s (5/2,1/2)
-	777987	-	54% 6s ^3D + 46% 6s ^1D	100% 6s (3/2,1/2)
$J = 3$				
378360a	378388	-28	100% 5s ^3D	100% 5s (5/2,1/2)
682036	682015	21	56% 5d ^3D + 32% 5d ^3F	80% 5d (5/2,3/2)
684331	684353	-22	41% 5d ^1F + 31% 5d ^3D	79% 5d (5/2,5/2)
692976	692933	43	72% 5d ^3G + 21% 5d ^1F	91% 5d (3/2,3/2)
700131	700215	-84	52% 5d ^3F + 34% 5d ^1F	95% 5d (3/2,5/2)
-	762884	-	100% 6s ^3D	100% 6s (5/2,1/2)
$J = 4$				
678541	678524	17	56% 5d ^3G + 42% 5d ^1G	97% 5d (5/2,3/2)
685764	685760	4	77% 5d ^3F + 19% 5d ^1G	96% 5d (5/2,5/2)
696240	696165	75	39% 5d ^1G + 40% 5d ^3G	97% 5d (3/2,5/2)
$J = 5$				
680206	680069	137	100% 5d ^3G	100% 5d (5/2,5/2)
Odd Configurations:				
$J = 0$				
516034a	516027	7	100% 5p ^3P	100% 5p (3/2,3/2)
-	856214	-	100% 5f ^3P	100% 5f (5/2,5/2)
$J = 1$				
505194	505116	78	80% 5p ^3P + 20% 5p ^3D	45% 5p (3/2,1/2)
515058a	515083	-25	82% 5p ^1P + 14% 5p ^3D	52% 5p (3/2,1/2)
525895a	525884	11	66% 5p ^3D + 18% 5p ^1P	84% 5p (3/2,3/2)
-	857564	-	88% 5f ^3P + 11% 5f ^3D	81% 5f (5/2,5/2)
-	868961	-	86% 5f ^3D + 11% 5f ^3P	42% 5f (3/2,5/2)
-	904447	-	76% 5f ^1P + 12% 4f ^1P	46% 5f (3/2,5/2)
$J = 2$				
489118a	489214	-96	78% 5p ^3P + 16% 5p ^3D	90% 5p (5/2,1/2)
504541a	504563	-22	87% 5p ^3F + 6% 5p ^3D	87% 5p (3/2,1/2)
512442a	512554	-112	66% 5p ^1D + 19% 5p ^3D	80% 5p (5/2,3/2)
528399a	528424	-25	58% 5p ^3D + 29% 5p ^1D	96% 5p (3/2,3/2)
-	859618	-	63% 5f ^3P + 24% 5f ^3D	69% 5f (5/2,7/2)
-	862905	-	39% 5f ^3F + 38% 5f ^1D	74% 5f (5/2,5/2)
-	873827	-	37% 5f ^3P + 36% 5f ^3D	85% 5f (3/2,7/2)
-	876887	-	61% 5f ^3F + 22% 5f ^1D	90% 5f (3/2,5/2)
$J = 3$				
492554a	492449	105	54% 5p ^3F + 33% 5p ^1F	98% 5p (5/2,1/2)
514852a	514739	113	73% 5p ^3D + 27% 5p ^1F	98% 5p (5/2,3/2)
523790a	523782	8	39% 5p ^1F + 46% 5p ^3F	98% 5p (3/2,3/2)
-	863109	-	48% 5f ^3D + 48% 5f ^3F	64% 5f (5/2,5/2)
-	866058	-	46% 5f ^1F + 21% 5f ^3G	63% 5f (5/2,7/2)
-	878106	-	40% 5f ^3F + 25% 5f ^3G	92% 5f (3/2,7/2)
-	879982	-	50% 5f ^3G + 43% 5f ^1F	93% 5f (3/2,5/2)
$J = 4$				
506971a	507014	-43	100% 5p ^3F	100% 5p (5/2,3/2)
-	863826	-	79% 5f ^3F + 17% 5f ^3G	75% 5f (5/2,7/2)
-	864560	-	46% 5f ^1G + 27% 5f ^3G	73% 5f (5/2,5/2)
-	874961	-	75% 5f ^3H + 15% 5f ^1G	93% 5f (3/2,5/2)
-	879214	-	45% 5f ^3G + 35% 5f ^1G	95% 5f (3/2,7/2)

Table VI. *Continued.*

$E(\text{exp})$	$E(\text{fit})$	ΔE	<i>LS</i> -coupling terms	<i>Jj</i> -coupling terms
<i>J</i> = 5				
–	861087	–	58% 5f ^3H + 41% 5f ^1H	98% 5f ($5/2, 5/2$)
–	865140	–	78% 5f ^3G + 17% 5f ^1H	98% 5f ($5/2, 7/2$)
–	876104	–	42% 5f ^1H + 37% 5f ^3H	98% 5f ($3/2, 7/2$)
<i>J</i> = 6				
–	860354	–	100% 5f ^3H	100% 5f ($5/2, 7/2$)

a – corrected energy value for a level previously known [8].

Table VII. Hartree–Fock (HF) and Least-Square-Fitted (LSF) energy parameters for Sb VI, Te VII and I VIII (cm^{-1}).

Parameter	Sb VI			Te VII			I VIII		
	HF	LSF	LSF/HF	HF	LSF	LSF/HF	HF	LSF	LSF/HF
Even configurations:									
$E_{\text{av}}(4\text{d}^{10})$	0	1639(57)	–	0	1607(71)	–	0	1575(84)	–
$E_{\text{av}}(5\text{s})$	250780	248635(29)	0.985	317504	314695(36)	0.986	389311	385867(43)	0.987
$\zeta(4\text{d})$	3974	4112(25)	1.035	4700	4861(31)	1.034	5504	5692(36)	1.034
$G0(4\text{d}, 5\text{s})$	16656	14526(264)	0.872	17406	15362(332)	0.883	18133	16173(406)	0.892
$E_{\text{av}}(5\text{d})$	477697	480194(14)	1.002	579908	581511(18)	1.000	687251	687858(27)	0.998
$\zeta(4\text{d})$	4010	4132(12)	1.030	4738	4883(16)	1.031	5544	5717(18)	1.031
$\zeta(5\text{d})$	507	619(17)	1.222	699	837(22)	1.197	925	1089(27)	1.177
$F2(4\text{d}, 5\text{d})$	21686	19281(132)	0.889	25482	22825(167)	0.896	29161	26219(202)	0.899
$F4(4\text{d}, 5\text{d})$	9673	9771(176)	1.010	11645	11931(223)	1.025	13584	14211(268)	1.046
$G0(4\text{d}, 5\text{d})$	5119	3944(9)	0.771	6019	4705(11)	0.782	6886	5445(13)	0.791
$G2(4\text{d}, 5\text{d})$	6327	5915(177)	0.935	7521	7105(214)	0.945	8675	8239(236)	0.950
$G4(4\text{d}, 5\text{d})$	5213	4874(146)	0.935	6250	5903(178)	0.945	7258	6892(197)	0.950
$E_{\text{av}}(6\text{s})$	517112	519180(29)	1.001	639342	640863(36)	1.000	769811	769836(fix)	0.998
$\zeta(4\text{d})$	4012	4144(23)	1.033	4742	4899(29)	1.033	5550	5710(fix)	1.033
$G0(4\text{d}, 6\text{s})$	4033	3641(282)	0.903	4420	4027(354)	0.911	4792	4409(fix)	0.920
St.Dev.		56			71			84	
Odd configurations:									
$E_{\text{av}}(5\text{p})$	345528	346467(24)	0.998	426729	425807(27)	0.994	512171	510424(27)	0.993
$\zeta(4\text{d})$	3988	4130(25)	1.036	4714	4880(27)	1.035	5518	5707(26)	1.034
$\zeta(5\text{p})$	6607	7446(49)	1.127	8493	9436(53)	1.111	10627	11648(52)	1.096
$F2(4\text{d}, 5\text{p})$	34728	29395(215)	0.846	38346	32704(248)	0.853	41806	36054(253)	0.862
$G1(4\text{d}, 5\text{p})$	11011	9899(84)	0.899	11882	10740(91)	0.904	12715	11567(89)	0.910
$G3(4\text{d}, 5\text{p})$	10412	9360(80)	0.899	11432	10333(90)	0.904	12400	11280(87)	0.910
$E_{\text{av}}(5\text{f})$	612143	613614(20)	1.000	737660	738421(21)	0.999	868702	868540(fix)	0.998
$\zeta(4\text{d})$	4000	4117(18)	1.029	4726	4819(20)	1.020	5533	5717(fix)	1.015
$\zeta(5\text{f})$	42	42(fix)	1.000	67	67(fix)	1.000	96	96(fix)	1.000
$F2(4\text{d}, 5\text{f})$	20025	171441(194)	0.856	22422	19324(214)	0.862	24366	21125(fix)	0.867
$F4(4\text{d}, 5\text{f})$	11591	10507(432)	0.906	12627	12118(482)	0.960	13194	13194(fix)	1.000
$G1(4\text{d}, 5\text{f})$	20972	11752(80)	0.560	21134	11731(79)	0.555	19788	11081(fix)	0.560
$G3(4\text{d}, 5\text{f})$	13157	11501(386)	0.874	13822	11734(413)	0.849	13540	11626(fix)	0.850
$G5(4\text{d}, 5\text{f})$	9297	8127(273)	0.874	9925	8425(296)	0.849	9891	8493(fix)	0.850
St.Dev.		81			90			89	

All the configuration interaction parameters were fixed at 0.85 HF values.

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