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Article

Energy Levels and Transition Data of Cs VI

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Abstract: Previously reported atomic data (spectral lines, wavelengths, energy levels, and transition probabilities) have been collected and systematically analyzed for the Cs VI. The present theoretical analysis is supported by extensive calculations made for Cs VI with a pseudo-relativistic Hartree–Fock (HFR) method together with the superposition of configuration interactions implemented in Cowan's codes. In this critical evaluation, we provided several possibly observable lines with Ritz-wavelengths, computed from the optimized energy levels, and theoretical transition probabilities with their estimated uncertainties. In addition, we provided the radiative transition parameters for several forbidden lines within the ground configuration $5s^25p^2$ of Cs VI.

Keywords: Atomic Spectra; cesium; energy levels; spectral lines; wavelengths; transition probabilities

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1. Introduction

In general, accurate atomic data on wavelengths, energy levels, transition probabilities, and oscillator strengths are needed to determine the atmospheric abundances of elements in any astrophysical source or object. By using these atomic data astronomers have for the first time identified elements heavier than hydrogen and helium in the atmospheres of white dwarfs. These were mostly traces of trans-iron elements (atomic numbers $Z \geq 30$) detected in the atmospheres of different hot white dwarfs G191-B2B, Feige 24, GD 246, HD 149499B, HZ 21, and RE 0503-289 [1–5]. Recently, Chayer et al. [6] identified the presence of cesium (Z = 55) by means of observing the several absorption lines of Cs IV-VI in the Far Ultraviolet Spectroscopic Explorer (FUSE) spectrum of the hot He-rich white dwarfs (spectral type DO) HD 149499B. The atomic structure and radiative transition parameters data for these atomic/ionic species, up to the ionization stage VII, were necessary to obtain accurate stellar atmospheric models for white dwarfs. Chayer et al. [6] calculated oscillator strengths for the bound–bound transitions of Cs IV-VI ion with AUTOSTRUCTURE and GRASP2K atomic structure codes. Both AUTOSTRUCTURE and GRASP2K calculations were performed with the same sets of atomic models, however, an extensive radiative transition parameter data set was provided from the AUTOSTRUCTURE calculations only, and the GRASP2K results were used for the comparison purpose. For Cs VI spectrum, these are for the $5s^25p^2 \rightarrow \{5s5p^3 + 5s^25p5d + 5s^25p6s\}$ transitions.

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In terms of experimental observations, the first study on Cs VI spectrum was made by Tauheed et al. [7]. They reported the levels of the ground configuration $5s^2 5p^2$ and those for the excited $5s5p^3$, $5s^2 5p5d$, and $5s^2 5p6s$ configurations, with the help of the spectra of cesium photographed in the 325–1400 Å wavelength region on a 3-m normal-incidence vacuum spectrograph at the Antigonish laboratory, Canada. The spectrograph was equipped with a 2400 lines/mm holographic grating giving a reciprocal dispersion of 1.385 Å/mm in the first order of wavelength. The cavities of the aluminum electrodes, filled with pure cesium carbonate and cesium nitrate salts, were used in a triggered spark source, which acts as a light source. A 30 kV trigger unit with a little current to initiate a 6 kV spark discharge in vacuum was used. Additionally, the wavelength information was also supplemented from the previously captured spectra of cesium, which were recorded on a 10.7-m normal incidence vacuum spectrograph at the National Institute of Standards and Technology (NIST), Gaithersburg. The Kodak short wave radiation (SWR) plates were used for all spectral exposures. The calibrations of spectrograms were carried out using the known lines of carbon, oxygen, and nitrogen present in the spectra as impurities, and they claimed an accuracy of 0.005 Å for strong and unperturbed lines in the entire wavelength region mentioned above. Tauheed et al. [7] findings were included in the latest spectral compilation of Cs I-LV provided by Sansonetti [8], and the same was also available in the NIST's Atomic Spectra Database (ASD) [9].

In the present work, our motivation is to provide an extensive atomic data set for the Cs VI spectrum, also to carry out critical evaluations for these data by means of their comparison with the existing data in the literature. In addition to these, we aim to compute radiative transition parameters for the forbidden lines between the levels of the ground configuration $5s^2 5p^2$.

2. Results and Discussion

The main results of our work on Cs VI are summarized in Tables 1 and 2. In Table 1 we present the classified lines of Cs VI with their radiative transition parameters and Table 2 describes the optimized energy levels with their LS compositions. The LS composition vectors are computed using the theoretical calculations made with Cowan's codes (see Section 2.2). Nevertheless, specific details of the current analysis are discussed in the sections below.

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Table 1. Classified lines of Cs VI.

$I_{obs.}$ [a] (arb. u.)	$\lambda_{obs.}$ [b] (Å)	σ [b] (cm^{-1})	Classification	λ_{Ritz} [b] (Å)	$\delta\lambda_{o-c}$ [c] (mÅ)	gA [d] (s^{-1})	CF [d]	Acc. [e]	gA_{prev} [f] (s^{-1})	Line Ref. [g]
			$5s^25p^2\,^3P_0-5s^25p6s\,^1P^\circ_1$	378.4639(21)		5.83e+07	0.00	E	7.71e+07	TW
22	396.746(5)	252050(3)	$5s^25p^2\,^3P_1-5s^25p6s\,^1P^\circ_1$	396.7443(22)	2	2.32e+09	0.58	D	9.66e+08	T91
38	401.968(5)	248776(3)	$5s^25p^2\,^3P_1-5s^25p6s\,^3P^\circ_2$	401.968(3)	0	1.75e+10	0.77	D+	1.12e+10	T91
15	405.518(5)	246598(3)	$5s^25p^2\,^3P_2-5s^25p6s\,^1P^\circ_1$	405.5171(23)	1	8.48e+09	0.16	D+	6.03e+09	T91
40	410.312(5)	243717(3)	$5s^25p^2\,^3P_0-5s^25p6s\,^3P^\circ_1$	410.310(3)	2	1.44e+10	0.45	D+	1.09e+10	T91
45	410.976(5)	243323(3)	$5s^25p^2\,^3P_2-5s^25p6s\,^3P^\circ_2$	410.976(3)	0	3.03e+10	0.76	D+	2.11e+10	T91
			$5s^25p^2\,^3P_0-5s^25p5d\,^1P^\circ_1$	431.007(3)		3.12e+07	0.00	E	1.10e+08	TW
38	431.883(5)	231544(3)	$5s^25p^2\,^3P_1-5s^25p6s\,^3P^\circ_1$	431.884(3)	-1	6.57e+09	0.54	D+	6.27e+09	T91
50	434.712(5)	230037(3)	$5s^25p^2\,^3P_1-5s^25p6s\,^3P^\circ_0$	434.712(5)	0	1.03e+10	0.69	D+	9.28e+09	T91
52	436.365(5)	229166(3)	$5s^25p^2\,^1D_2-5s^25p6s\,^1P^\circ_1$	436.365(3)	0	3.98e+10	0.69	C	3.33e+10	T91
57	442.298(5)	226092(3)	$5s^25p^2\,^3P_2-5s^25p6s\,^3P^\circ_1$	442.300(3)	-2	1.99e+10	0.50	D+	1.71e+10	T91
47	442.693(5)	225890(3)	$5s^25p^2\,^1D_2-5s^25p6s\,^3P^\circ_2$	442.693(3)	0	1.41e+10	0.75	D+	1.34e+10	T91
			$5s^25p^2\,^3P_1-5s^25p5d\,^1P^\circ_1$	454.875(3)		4.91e+08	0.03	D	3.66e+08	TW
25	466.447(5)	214386.6(23)	$5s^25p^2\,^3P_2-5s^25p5d\,^1P^\circ_1$	466.445(3)	2	2.29e+09	0.04	D+	2.41e+09	T91
			$5s^25p^2\,^3P_0-5s^25p5d\,^3P^\circ_1$	466.887(3)		4.24e+07	0.00	E	1.70e+08	TW
38	472.107(5)	211816.4(22)	$5s^25p^2\,^1S_0-5s^25p6s\,^1P^\circ_1$	472.109(3)	-2	1.82e+10	0.82	C	2.70e+10	T91
55	478.711(5)	208894.3(22)	$5s^25p^2\,^3P_2-5s^25p5d\,^1F^\circ_3$	478.709(3)	2	3.57e+10	0.13	C	3.00e+10	T91
			$5s^25p^2\,^1D_2-5s^25p6s\,^3P^\circ_1$	479.253(4)		4.92e+08	0.01	E	8.14e+07	TW
38	490.613(5)	203826.6(21)	$5s^25p^2\,^3P_1-5s^25p5d\,^3D^\circ_2$	490.612(3)	1	7.48e+09	0.04	D+	1.71e+10	T91
65	495.028(5)	202008.8(20)	$5s^25p^2\,^3P_1-5s^25p5d\,^3P^\circ_1$	495.024(3)	4	4.62e+10	0.51	C	4.43e+10	T91
55	498.127(5)	200752.0(20)	$5s^25p^2\,^3P_1-5s^25p5d\,^3P^\circ_0$	498.127(5)	0	2.50e+10	0.66	C	2.33e+10	T91
70	500.502(5)	199799.4(20)	$5s^25p^2\,^3P_0-5s^25p5d\,^3D^\circ_1$	500.5033(24)	-1	7.26e+10	0.50	C	7.14e+10	T91
58	504.097(5)	198374.5(20)	$5s^25p^2\,^3P_2-5s^25p5d\,^3D^\circ_2$	504.098(3)	-1	2.78e+10	0.13	C	3.98e+10	T91
66	506.020(5)	197620.6(20)	$5s^25p^2\,^3P_1-5s^25p5d\,^1D^\circ_2$	506.024(3)	-4	6.59e+10	0.71	C	6.94e+10	T91
			$5s^25p^2\,^1D_2-5s^25p5d\,^1P^\circ_1$	507.731(4)		2.71e+09	0.04	D+	3.68e+09	TW
48	508.757(5)	196557.5(19)	$5s^25p^2\,^3P_2-5s^25p5d\,^3P^\circ_1$	508.757(3)	0	2.03e+10	0.43	C	1.89e+10	T91
75	514.093(5)	194517.3(19)	$5s^25p^2\,^3P_2-5s^25p5d\,^3D^\circ_3$	514.090(3)	3	1.96e+11	0.71	C	1.93e+11	T91
50	514.241(5)	194461.4(19)	$5s^25p^2\,^3P_0-5s5p^3\,^1P^\circ_1$	514.2438(22)	-3	1.28e+10	0.17	D+	8.97e+09	T91
65	520.375(5)	192169.1(18)	$5s^25p^2\,^3P_2-5s^25p5d\,^1D^\circ_2$	520.383(3)	-8	6.53e+10	0.48	C	3.76e+10	T91
70	522.294(5)	191463.0(18)	$5s^25p^2\,^1D_2-5s^25p5d\,^1F^\circ_3$	522.296(4)	-2	2.06e+11	0.72	C	1.96e+11	T91
			$5s^25p^2\,^1S_0-5s^25p6s\,^3P^\circ_1$	522.717(5)		4.77e+09	0.28	D+	6.98e+09	TW

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78m(Cs V)	532.992(10)	187620(4)	$5s^25p^2\ ^3P_1$-$5s^25p5d\ ^3D^\circ_1$	532.980(2)	12	2.10e+10	0.23	C	1.66e+10	T91
70	539.366(5)	185402.9(17)	$5s^25p^2\ ^3P_1$-$5s^25p5d\ ^3P^\circ_2$	539.364(3)	2	7.43e+10	0.69	C	5.69e+10	T91
45	548.591(5)	182285.2(17)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^1P^\circ_1$	548.5891(21)	2	5.98e+09	0.14	D+	9.01e+09	T91
			$5s^25p^2\ ^3P_2$-$5s^25p5d\ ^3D^\circ_1$	548.933(3)		5.85e+08	0.01	D+	1.47e+09	TW
64	552.665(5)	180941.4(16)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3D^\circ_2$	552.665(3)	0	9.14e+10	0.65	C	7.36e+10	T91
63	555.703(5)	179952.2(16)	$5s^25p^2\ ^3P_2$-$5s^25p5d\ ^3P^\circ_2$	555.708(3)	-5	3.54e+10	0.21	C	4.51e+10	T91
55	556.777(5)	179605.1(16)	$5s^25p^2\ ^1S_0$-$5s^25p5d\ ^1P^\circ_1$	556.779(4)	-2	6.32e+10	0.58	C	5.31e+10	T91
45	558.268(5)	179125.4(16)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3P^\circ_1$	558.271(3)	-3	1.45e+10	0.59	C	1.44e+10	T91
52	564.697(5)	177086.1(16)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3D^\circ_3$	564.699(4)	-2	2.18e+10	0.14	C	2.02e+10	T91
8	565.503(5)	176833.7(16)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^1P^\circ_1$	565.5053(22)	-2	4.21e+08	0.00	D	4.44e+08	T91
52	569.332(5)	175644.4(15)	$5s^25p^2\ ^3P_0$-$5s5p^3\ ^3S^\circ_1$	569.333(3)	-1	8.72e+09	0.19	D+	8.67e+09	T91
50	572.310(5)	174730.5(15)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^1D^\circ_2$	572.301(3)	9	2.02e+10	0.17	C	3.02e+10	T91
72	589.477(5)	169641.9(14)	$5s^25p^2\ ^3P_2$-$5s^25p5d\ ^3F^\circ_3$	589.477(5)	0	1.50e+10	0.70	C	1.18e+10	T91
40	589.691(5)	169580.3(14)	$5s^25p^2\ ^3P_1$-$5s^25p5d\ ^3F^\circ_2$	589.695(3)	-4	2.70e+09	0.60	D+	2.31e+09	T91
42	607.020(5)	164739.2(14)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3D^\circ_1$	607.022(3)	-2	6.19e+09	0.20	D+	4.72e+09	T91
65	609.285(5)	164126.8(13)	$5s^25p^2\ ^3P_2$-$5s^25p5d\ ^3F^\circ_2$	609.287(3)	-2	5.14e+09	0.39	D+	4.22e+09	T91
72	611.735(5)	163469.5(13)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^3S^\circ_1$	611.735(3)	0	1.62e+10	0.34	C	1.45e+10	T91
55	615.320(5)	162517.1(13)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3P^\circ_2$	615.317(3)	3	8.90e+09	0.08	C	1.10e+10	T91
			$5s^25p^2\ ^1S_0$-$5s^25p5d\ ^3P^\circ_1$	618.145(5)		4.57e+07	0.00	E	5.68e+05	TW
75	627.360(5)	159398.1(13)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^1P^\circ_1$	627.352(3)	8	2.72e+10	0.37	C	2.65e+10	T91
82	632.846(5)	158016.3(12)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^3S^\circ_1$	632.844(3)	2	3.89e+10	0.50	C	3.60e+10	T91
32	638.762(5)	156552.8(12)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^1D^\circ_2$	638.753(3)	9	5.88e+08	0.04	D	5.08e+08	T91
68	648.526(5)	154195.8(12)	$5s^25p^2\ ^3P_0$-$5s5p^3\ ^3P^\circ_1$	648.518(3)	8	2.04e+09	0.05	D+	1.77e+09	T91
			$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3F^\circ_3$	656.992(6)		8.23e+05	0.00	E	3.26e+06	TW
			$5s^25p^2\ ^3P_2$-$5s5p^3\ ^1D^\circ_2$	661.804(3)		2.91e+07	0.00	E	6.77e+06	TW
62	678.479(5)	147388.5(11)	$5s^25p^2\ ^1S_0$-$5s^25p5d\ ^3D^\circ_1$	678.479(4)	0	2.02e+08	0.01	E	5.38e+06	T91
60	681.699(5)	146692.3(11)	$5s^25p^2\ ^1D_2$-$5s^25p5d\ ^3F^\circ_2$	681.694(3)	5	3.27e+09	0.28	D+	2.71e+09	T91
			$5s^25p^2\ ^3P_1$-$5s5p^3\ ^3P^\circ_2$	701.260(5)		3.07e+07	0.00	E	4.58e+07	TW
80	703.973(5)	142050.9(10)	$5s^25p^2\ ^1S_0$-$5s5p^3\ ^1P^\circ_1$	703.978(4)	-5	3.83e+09	0.08	D+	2.78e+09	T91
25	704.104(5)	142024.5(10)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^3P^\circ_1$	704.110(3)	-6	5.84e+09	0.19	D+	4.50e+09	T91
80bl(Cs VII)	711.313(10)	140585.1(20)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^3S^\circ_1$	711.319(4)	-6	4.69e+08	0.01	D	1.40e+08	T91
25	711.953(5)	140458.7(10)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^3P^\circ_0$	711.953(5)	0	2.12e+09	0.18	D+	1.65e+09	T91
78	729.141(5)	137147.7(9)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^3P^\circ_2$	729.141(5)	0	9.94e+09	0.13	C	6.79e+09	T91

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80	732.217(5)	136571.5(9)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^3P^\circ_1$	732.223(3)	-6	2.11e+08	0.01	D	1.42e+08	T91
88	748.109(5)	133670.4(9)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^1D^\circ_2$	748.115(4)	-6	8.34e+09	0.11	D+	4.33e+09	T91
72	758.917(5)	131766.7(9)	$5s^25p^2\ ^3P_0$-$5s5p^3\ ^3D^\circ_1$	758.921(4)	-4	3.48e+09	0.12	D+	2.68e+09	T91
			$5s^25p^2\ ^1S_0$-$5s5p^3\ ^3S^\circ_1$	811.466(6)		5.17e+08	0.04	D	3.65e+08	TW
52	827.035(5)	120913.9(7)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^3D^\circ_2$	827.037(3)	-2	4.03e+09	0.11	D+	2.81e+09	T91
50	830.465(5)	120414.5(7)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^3D^\circ_3$	830.464(3)	1	3.19e+09	0.09	D+	2.04e+09	T91
			$5s^25p^2\ ^1D_2$-$5s5p^3\ ^3P^\circ_2$	835.320(7)		3.82e+08	0.01	D	2.01e+08	TW
61	836.190(5)	119590.0(7)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^3D^\circ_1$	836.180(3)	10	4.23e+07	0.00	E	8.20e+06	T91
			$5s^25p^2\ ^1D_2$-$5s5p^3\ ^3P^\circ_1$	839.367(4)		3.79e+06	0.00	E	4.62e+04	TW
30	866.096(5)	115460.6(7)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^3D^\circ_2$	866.095(3)	1	4.79e+07	0.00	D	5.06e+07	T91
34	876.127(5)	114138.7(7)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^3D^\circ_1$	876.127(3)	0	2.55e+08	0.05	D	2.52e+08	T91
54	971.046(5)	102981.7(5)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^3D^\circ_3$	971.047(4)	-1	1.48e+09	0.11	D+	9.46e+08	T91
4	982.444(5)	101787.0(5)	$5s^25p^2\ ^1S_0$-$5s5p^3\ ^3P^\circ_1$	982.441(4)	3	1.46e+08	0.08	D	1.24e+08	T91
75	1020.118(5)	98027.9(5)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^3D^\circ_2$	1020.118(4)	0	6.27e+07	0.01	D	2.85e+07	T91
22	1034.060(5)	96706.2(5)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^3D^\circ_1$	1034.065(4)	-5	1.38e+08	0.05	D	1.49e+08	T91
75	1055.929(5)	94703.3(4)	$5s^25p^2\ ^3P_1$-$5s5p^3\ ^5S^\circ_2$	1055.936(4)	-7	1.67e+08	0.21	D	1.44e+08	T91
73	1120.452(5)	89249.7(4)	$5s^25p^2\ ^3P_2$-$5s5p^3\ ^5S^\circ_2$	1120.450(4)	2	1.43e+08	0.15	D	1.27e+08	T91
			$5s^25p^2\ ^1S_0$-$5s5p^3\ ^3D^\circ_1$	1260.151(11)		9.42e+06	0.01	E	4.85e+06	TW
5	1392.432(5)	71816.8(3)	$5s^25p^2\ ^1D_2$-$5s5p^3\ ^5S^\circ_2$	1392.430(4)	2	1.09e+07	0.03	D	9.74e+06	T91

[a] Observed relative intensities in arbitrary units, which were taken from T91–Tauheed et al. [7], character of the observed line: bl–blended by a close line, m–masked by a stronger neighboring line. [b] Observed and Ritz wavelengths (in Å) are given in vacuum for all observed wavenumbers (σ) expressed in cm^{-1} unit. The quantity given in parentheses is the uncertainty in the last digit. [c] Difference between the observed and Ritz wavelengths in mÅ, and 1m Å= 10^{-3} Å. [d] Weighted transition probability (gA-value) and absolute cancellation factor from the present HFR-B calculations (see Section 2.2). [e] Accuracy code of the gA-value explained in Section 2.2. [f] gA-values obtained from the A-values reported previously by Chayer et al. [6]. [g] Line reference: T91-Tauheed et al. [7], TW–this work.

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Table 2. Optimized energy levels of Cs VI.

Level	Energy [a] (cm^{-1})	Unc. [b] (cm^{-1})	Leading Compositions [c] P1	P2	Comp2	P3	Comp3	ΔE_{o-c} [d] (cm^{-1})	No. of Lines [e]
$5s^25p^2\ ^3P_0$	0.0	0.8	87	12	$5s^25p^2\ ^1S$			4	6
$5s^25p^2\ ^3P_1$	12174.5	0.5	98					0	16
$5s^25p^2\ ^3P_2$	17627.3	0.3	62	36	$5s^25p^2\ ^1D$			-8	18
$5s^25p^2\ ^1D_2$	35060.26	0.20	61	36	$5s^25p^2\ ^3P$			5	17
$5s^25p^2\ ^1S_0$	52410.4	0.5	86	12	$5s^25p^2\ ^3P$			-1	5
$5s5p^3\ ^5S^\circ_2$	106877.18	0.24	91	7	$5s5p^3\ ^3P^\circ$			26	3
$5s5p^3\ ^3D^\circ_1$	131766.0	0.5	74	12	$5s5p^3\ ^3P^\circ$	7	$5s^25p5d\ ^3D^\circ$	-260	4
$5s5p^3\ ^3D^\circ_2$	133088.1	0.4	72	14	$5s5p^3\ ^3P^\circ$	6	$5s^25p5d\ ^3D^\circ$	-63	3
$5s5p^3\ ^3D^\circ_3$	138041.9	0.4	91	8	$5s^25p5d\ ^3D^\circ$			112	2
$5s5p^3\ ^3P^\circ_0$	152633.2	1.0	92	7	$5s^25p5d\ ^3P^\circ$			-99	1
$5s5p^3\ ^3P^\circ_1$	154197.7	0.5	75	12	$5s5p^3\ ^3D^\circ$	5	$5s^25p5d\ ^3P^\circ$	88	4
$5s5p^3\ ^3P^\circ_2$	154774.9	0.9	42	23	$5s5p^3\ ^1D^\circ$	14	$5s5p^3\ ^3D^\circ$	130	1
$5s5p^3\ ^1D^\circ_2$	168729.5	1.3	34	27	$5s5p^3\ ^3P^\circ$	27	$5s^25p5d\ ^1D^\circ$	196	2
$5s5p^3\ ^3S^\circ_1$	175644.1	0.8	64	27	$5s5p^3\ ^1P^\circ$			-9	4
$5s^25p5d\ ^3F^\circ_2$	181753.6	0.9	86	8	$5s5p^3\ ^1D^\circ$			95	3
$5s^25p5d\ ^3F^\circ_3$	187269.2	1.4	89	5	$5s^25p5d\ ^3D^\circ$			-205	1
$5s5p^3\ ^1P^\circ_1$	194460.3	0.9	48	24	$5s5p^3\ ^3S^\circ$	15	$5s^25p5d\ ^1P^\circ$	-112	5
$5s^25p5d\ ^3P^\circ_2$	197578.0	1.0	45	22	$5s^25p5d\ ^3D^\circ$	15	$5s^25p5d\ ^1D^\circ$	105	3
$5s^25p5d\ ^3F^\circ_4$	(199500)	(400)	98						
$5s^25p5d\ ^3D^\circ_1$	199798.9	0.8	60	16	$5s^25p5d\ ^3P^\circ$	8	$5s5p^3\ ^1P^\circ$	98	4
$5s^25p5d\ ^1D^\circ_2$	209793.6	1.8	35	37	$5s^25p5d\ ^3D^\circ$	15	$5s5p^3\ ^1D^\circ$	-90	3
$5s^25p5d\ ^3D^\circ_3$	212145.7	1.4	76	7	$5s^25p5d\ ^3F^\circ$	7	$5s^25p5d\ ^1F^\circ$	-46	2
$5s^25p5d\ ^3P^\circ_0$	212926.5	2.0	91	6	$5s5p^3\ ^3P^\circ$			-34	1
$5s^25p5d\ ^3P^\circ_1$	214184.8	1.2	66	21	$5s^25p5d\ ^3D^\circ$	6	$5s5p^3\ ^3P^\circ$	24	3
$5s^25p5d\ ^3D^\circ_2$	216001.6	1.1	27	44	$5s^25p5d\ ^3P^\circ$	11	$5s^25p5d\ ^1D^\circ$	42	3
$5s^25p5d\ ^1F^\circ_3$	226522.6	1.5	87	9	$5s^25p5d\ ^3D^\circ$			-76	2
$5s^25p5d\ ^1P^\circ_1$	232015.0	1.4	74	10	$5s5p^3\ ^1P^\circ$	6	$5s^25p5d\ ^3D^\circ$	84	2
$5s^25p6s\ ^3P^\circ_0$	242212	3	98					98	1
$5s^25p6s\ ^3P^\circ_1$	243718.4	1.6	73	21	$5s^25p6s\ ^1P^\circ$			16	3
$5s^25p6s\ ^3P^\circ_2$	260950.5	1.6	98					-109	3
$5s^25p6s\ ^1P^\circ_1$	264226.0	1.4	73	23	$5s^25p6s\ ^3P^\circ$			-9	4

[a] Optimized energy values obtained using LOPT code [10]. The value given in parentheses and its uncertainty are the theoretical ones from the LSF of Cowan's code (see 2.2). [b] Uncertainties resulting from the level optimization procedure is the D1 uncertainty (D1 is close to the minimum estimated dispersion relative to any other term; see further detail in ref. [10]). [c] The LS-coupling percentage compositions determined in this work were made by parametric least-squares fitting with Cowan's codes (see text), wherein P1 refers to the first percentage value of the configuration and term given in the first column of the table. The remaining percentage (P2, P3) values are provided with their corresponding components. [d] Differences between observed and calculated energies in the parametric least-squares fitting. Blank for unobserved levels. [e] Number of observed lines determining the level in the level optimization.

2.1. Optimization of Energy Levels

First, we collected all experimentally observed wavelength data of Cs VI in the literature [7]. Those are for the $5s^25p^2$–$5s5p^3$, $5s^25p^2$–$5s^25p5d$, and $5s^25p^2$–$5s^25p6s$ transition arrays. The energy values of the levels involved in transition were computed from their observed spectral line data, i.e., transition wavelengths with uncertainties. In this regard, we used a least-squares level optimization code, 'LOPT' [10]. The transition wavelength, its measurement uncertainty, and unique lower and upper-level designation for each transition were necessary data inputs to the "LOPT-code". In the initial stage of the optimization, only observed wavelengths of Cs VI reported by Tauheed et al. [7] with an uncertainty of 0.005 Å were included as an input to the code. The levels involved were supported by 67 observed lines, resulted with their optimized energy values and uncertainties (see Table 2). For each of the observed wavelengths, their counterpart (precise) Ritz wavelengths with uncertainties were determined from the optimized energy levels. Furthermore, we use the optimized energy levels

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to derive the accurate Ritz wavelengths for several possibly observable lines of Cs VI (see Table 1) and for the forbidden transitions within the ground configuration (see Section 2.3).

2.2. Theoretical Calculations and Transition Probabilities

To support the present experimental observations, theoretical calculations were made within the framework of a pseudo-relativistic Hartree-Fock (HFR) approach with the superposition of interacting configurations, which implemented in Cowan's suite of codes [11]. Two sets of atomic models with varying configuration types, described in Table 3, were considered in this work. In both models the Slater's parameters were kept at 85% of the HFR-value for the F^k, 80% for the G^k, 70% for R^k, and the E_{av} and $\zeta_{n,l}$ parameters were fixed at 100% of their HFR-values. A least-squares parametric fitting (LSF) was performed to minimize the differences between the observed and theoretical energy values in the Cs VI. The standard deviation (SD) of the parametric LSF is given in Table 3 together with the total number of known levels and the number of free parameters involved in the fitting process, the latter is given in curly brackets. All fitted parameters together with their values in the LSF of the present HFR-B model is supplemented by us in Table A1. Using these fitted energy parameters, the transition probabilities (TPs or gA-values) were re-calculated for Cs VI. The obtained gA-values from the HFR-B model along with their cancellation factor ($|CF|$-values) are given in Table 1. The LS percentage compositions of the observed energy levels from the present HFR-B calculations are given in Table 2. As we compared our present LS percentage compositions with previously reported LS percentage compositions in references [7,8] a good matching was found. The LS assignments for most of the levels were found to be good without any ambiguity in our extensive calculation except for two levels of $5s^25p5d$ configuration:- $^1D_2$ at 209793.6 cm^{-1} and $^3D_2$ at 216001.6 cm^{-1}, which were assigned to their second-largest LS percentage component (see Table 2). This observation is in agreement with those made previously by Tauheed et al. [7].

Table 3. Configurations used in HFR models of Cs VI.

Even Parity	Odd Parity
Model: HFR-A	
$5s^25p^2$, $5p^4$	$5s5p^3$
$5s^25p6p$	$5s^25p\{(5,6)d + (6,7)s\}$
$5s5p^2\{(5,6)d + (6,7)s\}$	$5s5p^26p$
$5p^36p$	$5p^3\{(5,6)d + (6,7)s\}$
$5s^25d^2$, $5s^26s^2$, $5s^25d6s$	$5s5p5d^2$, $5s5p6s^2$
$5p^25d^2$, $5p^26s^2$, $5p^25d6s$	$5s5p5d6s$
....	....
No. of Levels[a] = 5{4}	No. of Levels[a] = 25{13}
SD = 15 cm^{-1}	SD = 276 cm^{-1}
Model: HFR-B	
$5s^25p^2$, $5p^4$	$5s5p^3$
$5s^25pnl$ $(n \leq 10, l = p, f)$	$5s^25pnl$ $(n \leq 10, l = s, d)$
$5s5p^2nl$ $(n \leq 8, l = s, d)$	$5s5p^2nl$ $(n \leq 8, l = p, f)$
$5p^3nl$ $(n \leq 10, l = p, f)$	$5p^3nl$ $(n \leq 10, l = s, d)$
$5s^24f^2$, $5s^25d^2$, $5s^26s^2$, $5s^26p^2$	
$5s^25d6s$, $5p^25d6s$, $5p^25d^2$	$5s5p5d^2$, $5s5p6s^2$
$5p^26s^2$, $5p^24f^2$, $5s5p5d4f$	$5s5p4f^2$, $5s5p5d6s$
....	....
No. of Levels[a] = 5{4}	No. of Levels[a] = 25{13}
SD = 10 cm^{-1}	SD = 155 cm^{-1}

[a] Total number of known levels and the number of free parameters in the LSF, the latter quantity is given in parentheses.

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Our main purpose of employing two different models – HFR-A and HFR-B with varying configuration types – was to compute and compare the transition probabilities data. Accordingly to compare and estimate the uncertainties of the transition probabilities with those reported by Chayer et al. [6] for the transition $5s^25p^2 \rightarrow \{5s5p^3 + 5s^25p5d + 5s^25p6s\}$ arrays in Cs VI. In their recent work, Chayer et al. used the multiconfiguration Breit-Pauli (MCBP) method to compute the A-values of C IV-VI. The MCBP method was implemented in the AUTOSTRUCTURE atomic structure code [12,13]. The configuration sets included in our HFR-A calculations are the same as those used in the MCBP calculations for Cs VI by Chayer et al., whereas those in our HFR-B model are more extensive in terms of the number of interacting configuration sets included in these calculations (see Table 3). Two types of comparison were employed in this work:- i) a qualitative scheme using gA-values and ii) a quantitative scheme, described in refs. [14–17], based on dS-values. The results of these comparisons were illustrated in Figure 1. The agreement between gA-values obtained from the present HFR-A and HFR-B calculations is shown in Figure 1(a), and their comparison of corresponding S-values given in Figure 1(b). The latter dS comparison shows gross disagreements within 26% for HFR-A and HFR-B models. Indeed the uncertainty for 56 strong lines with S$\geq$0.10 AU (atomic units) was 9% and 47% for the remaining 27 weak lines (see Figure 1(a)). All of these weak lines are strongly affected by cancellations, i.e., those having $|CF| < 0.10$, as a consequence, their S-values or gA-values are less reliable in comparison to those unaffected ones with $|CF| \geq 0.10$ (see details ref. [11]). There is an alternate method to derive the uncertainty for each S-value by means of generating different sets of LSF calculations with varying parameters within their uncertainty bounds. We use this method to estimate the uncertainty for each of the S-values obtained from the present HFR-B model. A total of six sets of LSF calculations were performed with varying parameters, and SDs of their S-values were computed and the same were taken to be an estimator for uncertainties in S-values. It should be noted that these SDs served as internal uncertainties for S-values obtained from the present HFR-B model, therefore, they represent as error bars in our final comparison model (see Figure 1(d)). Nonetheless, the strong lines with S$\geq$0.10 AU have an average uncertainty 5% and 18% for the other weak lines. The S-values which suffer strong cancellations have an average uncertainty of about 18% and unaffected ones were accurate within 3%. Our final comparison model for gA-values from the HFR-B with those from the MCBP method by Chayer et al. [6] is shown in figure 1(c), and their corresponding S-values comparison is given in Figure 1(d). To obtain more reliable estimates, this comparison model was selected, and its main results are summarized here. Though the gross disagreements between two sets of S-values fall within 160%, the strong lines with S$\geq$1 AU are accurate within 24%, 34% for the lines within the mid-range of S$\in$[0.1, 1) AU, it is about 50% for weak lines with S$\in$[0.01, 0.1) AU, and the remaining very weak lines are accurate within two to three orders of magnitude. It has been found that most of the cancellation affected (25 out of 33) transitions from the HFR-B model with $|CF| < 0.10$ fall in the category of accuracy >50%, and they are also the weak lines with S < 0.10 AU. All transitions listed Table 1 were provided with gA-values and their uncertainty codes and $|CF|$-values. The uncertainty codes are C types with an accuracy $\leq$25%, D+ with $\leq$40%, D with $\leq$50%, and those E types with an accuracy >50%.

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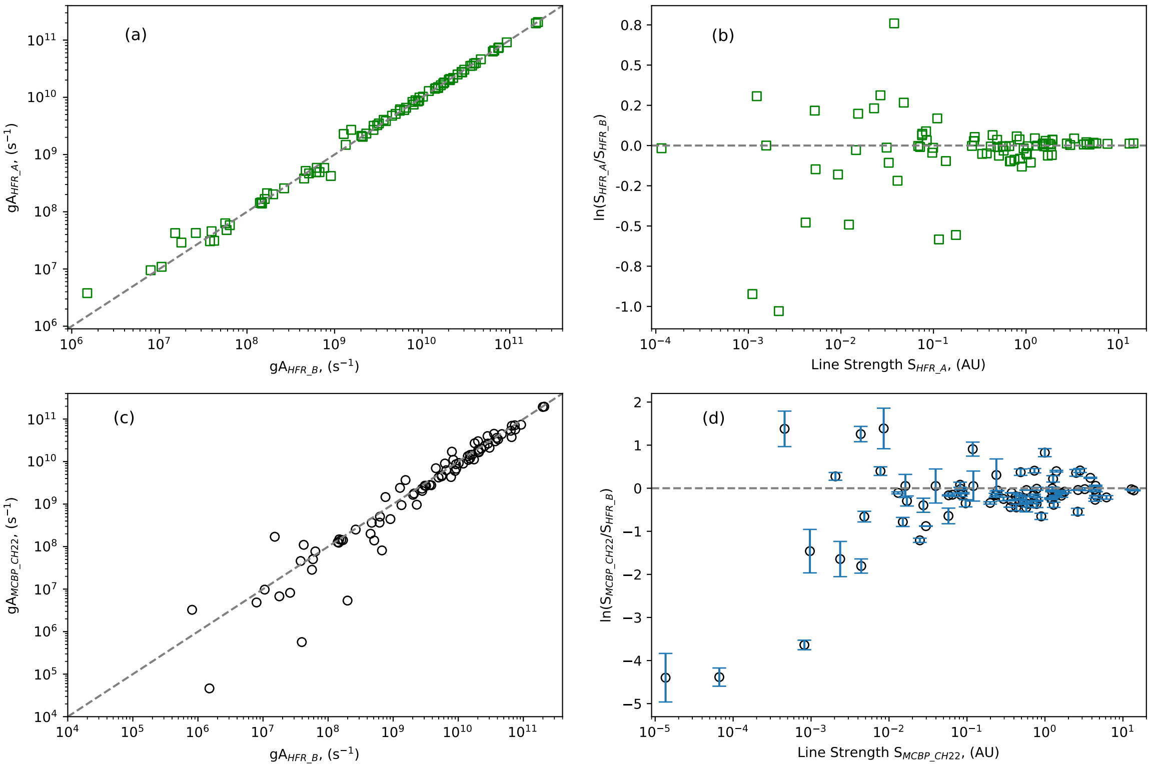

Figure 1. Comparison plots for gA-values and S-values: (a),(b) computed with our HFR-A and HFR-B models and (c),(d) obtained from HFR-B with those of the MCBP model by Chayer et al. [6]. The Error bars in panel (d) represent the internal uncertainties of S-values obtained from the HFR-B model (see the text)

Curtis [18] previously determined semi-empirical branching fraction (BF) for lines in the $5s^25p^2$-$5s^25p6s$ transition array in Sn I isoelectronic sequence (Sn I-Cs VI) by (least-squares) adjusting energy values of the levels involved, thereby obtained the optimized values for F^2 and ζ_{pp} parameters for $5s^25p^2$ and G^1 and ζ_p for $5s^25p6s$ configuration, followed by determination of the mixing angles to compute the relative transition rates (A-values). Recently, Chayer et al. [6] also reported the branching fractions (BFs), which computed from the MCBP A-values, for $5s^25p^2 - 5s^25p6s$ transitions. The comparison of these two BF data sets with 13 lines shows a gross disagreement within 300%. The most deviated data points were for the following (mostly) inter-combination transitions: 5p^2 ^{1}S$_0$–5p6s ^{1,3}P$^\circ_1$, 5p^2 ^{3}P$_0$–5p6s ^{1}P$^\circ_1$, 5p^2 ^{3}P$_1$–5p6s ^{1}P$^\circ_1$, and 5p^2 ^{1}D$_2$–5p6s ^{3}P$^\circ_1$. This indicates that either the singlet-triplet mixing angles were not computed accurately in the calculations of Curtis [18] or partly some of the MCBP A-values of Chayer et al. [6] are largely uncertain for the $5s^25p^2$-$5s^25p6s$ transitions. To investigate this, we compute the BFs for these transitions from their corresponding gA-values of the present HFR-A and HFR-B models. A good agreement (within 10%) between BF-values obtained from HFR-A and HFR-B models was found for the $5s^25p^2$-$5s^25p6s$ transitions. Nevertheless, the BFs from the extensive HFR-B model was selected by us for their consequent comparison with those of Curtis [18] and Chayer et al. [6]. The results of this comparison are shown in Figure 2(a). It has been found that the general agreement between BFs of HFR-B and those of Curtis is good except for two inter-combinations 5p^2 ^{1}S$_0$–5p6s ^{3}P$^\circ_1$ and 5p^2 ^{3}P$_0$–5p6s ^{1}P$^\circ_1$ transitions, which shows that the computed singlet-triplet mixing angles alone were inadequate to define A-values for these transitions by Curtis [18]. It should be noted that the intermediate coupling semi-empirical approaches of Curtis [18] are valid in the absence of configuration interaction. However, this assumption is not fully true for complex atomic systems, including Cs VI, in which both intra- and inter-configuration interactions are significant and particularly for the spin-forbidden inter-combination lines which are more sensitive to cancellation effects [19]. Figure 2(b) shows the gross comparison of the BFs from the present HFR-B

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model with those from the MCBP calculations of Chayer et al. [6] the transition $5s^25p^2 \rightarrow \{5s5p^3 + 5s^25p5d + 5s^25p6s\}$ arrays, and their overall agreement is found to be reasonably good.

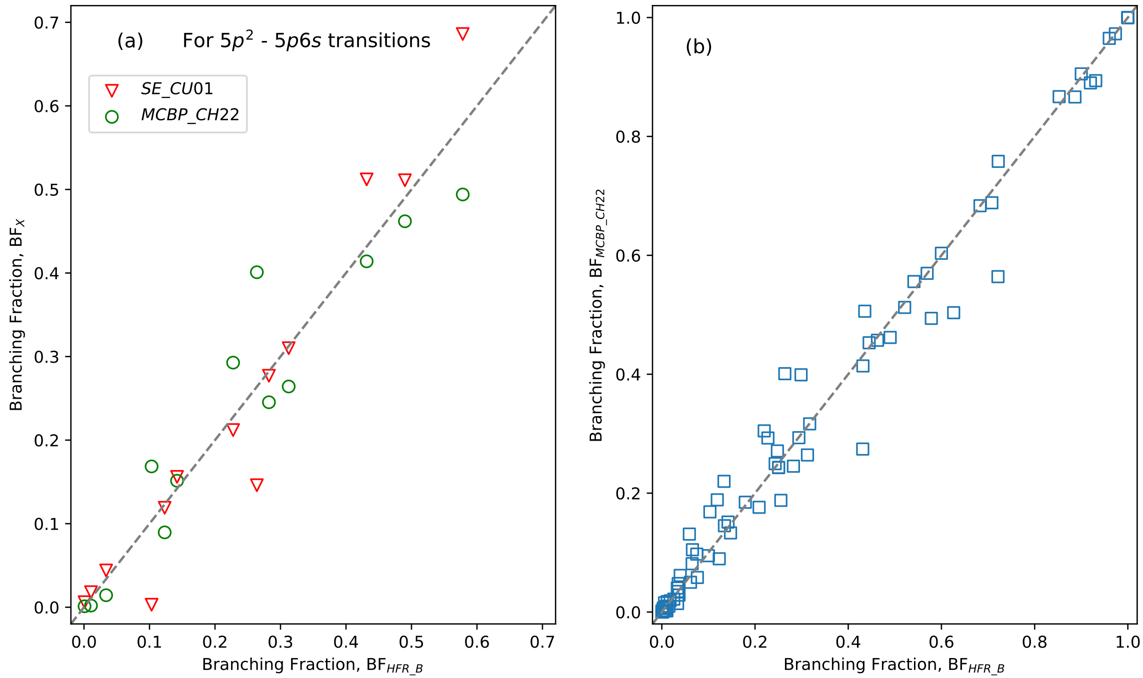

Figure 2. A comparison of (a) theoretical branching fractions BF_{HFR_B} obtained from the gA-values of the present HFR-B model with those semi-empirical BF_{SE_CU01}-values (in triangles) reported by Curtis [18] and with those theoretical BF_{MCBP_CH22} (in circles) computed from the MCBP A-values of Chayer et al. [6] for the selected $5s^25p^2 - 5s^25p6s$ transitions (b) theoretical BF_{HFR_B} with those BF_{MCBP_CH22} for the transition $5s^25p^2 \rightarrow \{5s5p^3 + 5s^25p5d + 5s^25p6s\}$ arrays (see the text).

2.3. Radiative parameters for transitions within the ground configuration

Biemont et al. [20] reported energy levels and radiative transition probabilities for states within the $5s^25p^k(k = 1 - 5)$ configurations of atoms and ions in the indium, tin, antimony, tellurium, and iodine isoelectronic sequences. These transitions are astrophysically important forbidden types having magnetic-dipole (M1) and/or electric-quadrupole (E2) components. For Cs VI spectrum, Biemont et al. [20] reported 3 M1 and 4 E2 transitions within the states of the ground configuration $5s^25p^2$. We also made a separate HFR calculations [11] with the even parity configurations in our HFR-B model. Our calculations are more extensive than the previous one made by Biemont et al. [20] for Cs VI. The obtained line parameters for 5 M1 and 7 E2 transitions of Cs VI are summarized in Table 4. To estimate the uncertainties of the presently obtained A-values, we performed a Monte Carlo technique suggested by Kramida [21]. This method evaluates the uncertainties of A-values by randomly varying the Slaters parameters of the known configurations included in the LSF. A total of 20 trials were made to estimate the uncertainties (%SD) of A-values of the transitions within the ground configuration and those are also given in Table 4.

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Table 4. Radiative rates for forbidden lines within the levels of ground $5s^2 5p^2$ configuration in Cs VI.

Transitions	This Work				Previous Work [d]		
	λ_{Ritz} [a] (Å)	A_{M1} [b] (s^{-1})	A_{E2} [b] (s^{-1})	%SD [c]	A_{M1} (s^{-1})	A_{E2} (s^{-1})	BF_{abs} [f]
$^3P_1$–$^1S_0$	2484.59(4)	4.170e+02		0.15			0.947
$^3P_0$–$^1D_2$	2851.39(5)		1.29e-02	3.00		1.511e-02	0.000
$^3P_2$–$^1S_0$	2874.12(5)		2.096e+01	0.30			0.048
$^3P_1$–$^1D_2$	4368.30(6)	6.032e+01	6.001e-01	0.20	5.996e+01	5.768e-01	0.545
$^3P_0$–$^3P_2$	5671.44(21)		2.6035e-01	0.04		2.542e-01	0.159
$^3P_2$–$^1D_2$	5734.67(10)	5.027e+01	6.655e-01	0.08			0.455
$^1D_2$–$^1S_0$	5762.04(21)		2.4906e+00	0.08			0.006
$^3P_0$–$^3P_1$	8211.6(5)	2.8743e+01		0.02	2.884e+01		1.000
$^3P_1$–$^3P_2$	18334.2(12)	1.3804e+00	7.889e-04	0.12	1.406e+00	7.896e-04	0.841

[a] Ritz wavelengths (in standard air [22]) and quantity given in parentheses is the uncertainty in the last digit. Wavelength uncertainties are determined in the level optimization procedure (see Section 2.1). [b] The scaled A-values for M1 and E2 components from the present HFR-B calculations (see Section 2.3). The scaling was carried out with the help of experimental transition energies computed from Table 2. [c] Uncertainties (%SD) of A-values for M1 and E2 components, obtained using the Monte Carlo method (see the text). [d] A-values for M1 and E2 components previously reported by Biemont et al. [20]. [f] Absolute branching fractions for the spectral lines are calculated from the present A-values given in columns 3 & 4.

3. Conclusion

In this work, a thorough critical analysis of the Cs VI spectrum has been carried out with the help of extensive HFR calculations made by us using Cowan's codes. This compilation provided a set of optimized energy levels (Table 2) of Cs VI ion with their uncertainties, as well as observed and Ritz wavelengths with their uncertainties for the levels involved. To the best of our knowledge, the accurate Ritz wavelengths with their uncertainties for this spectrum have been derived for the first time, and the same has been presented in Table 1 along with gA-values. The uncertainty estimates have been made of gA-values from their comparison with the previous data [6]. In addition, we report the radiative parameters for the forbidden (M1 and E2) lines within the ground configuration $5s^2 5p^2$ of Cs VI.

Author Contributions: Conceptualization, K.H.; methodology, K.H.; software, A.H., K.H. and A.T.; validation, A.H. and K.H.; formal analysis, A.H. and K.H.; investigation, A.H. and K.H.; data curation, K.H.; writing—original draft preparation, A.H. and K.H.; writing—review and editing, K.H. and A.T.; visualization, A.H. and K.H.; supervision, K.H. and A.T.; project administration, K.H.. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Supplementary Data

Table A1. Least-Squares Fitted Parmeters of Cs VI.

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p^2	E_{av}	30641.00	5		29620.80	1.034
5p^2	$F^2(5p, 5p)$	49951.70	58	1	59884.47	0.834
5p^2	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^2	$\zeta(5p)$	12115.30	9	2	11468.40	1.056
5p6p	E_{av}	308771.90	fixed		308771.90	1.000
5p6p	$\zeta(6p)$	12904.90	10	2	12215.80	1.056
5p6p	$\zeta(p)$	3534.10	fixed		3534.10	1.000
5p6p	$F^2(6p, p)$	19280.70	fixed		22683.18	0.850
5p6p	$G^0(6p, p)$	3798.40	fixed		4748.00	0.800

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p6p	$G^2(6p,p)$	5116.30	fixed		6395.38	0.800
5p7p	E_{av}	415145.50	fixed		415145.50	1.000
5p7p	$\zeta(7p)$	12974.90	10	2	12282.10	1.056
5p7p	$\zeta(p)$	1704.40	fixed		1704.40	1.000
5p7p	$F^2(7p,p)$	8550.90	fixed		10059.88	0.850
5p7p	$G^0(7p,p)$	1317.70	fixed		1647.13	0.800
5p7p	$G^2(7p,p)$	1957.20	fixed		2446.50	0.800
5p8p	E_{av}	469375.40	fixed		469375.40	1.000
5p8p	$\zeta(8p)$	13005.60	10	2	12311.10	1.056
5p8p	$\zeta(p)$	958.40	fixed		958.40	1.000
5p8p	$F^2(8p,p)$	4519.80	fixed		5317.41	0.850
5p8p	$G^0(8p,p)$	641.30	fixed		801.63	0.800
5p8p	$G^2(8p,p)$	991.90	fixed		1239.88	0.800
5p9p	E_{av}	501140.00	fixed		501140.00	1.000
5p9p	$\zeta(9p)$	13020.60	10	2	12325.30	1.056
5p9p	$\zeta(p)$	594.00	fixed		594.00	1.000
5p9p	$F^2(9p,p)$	2686.60	fixed		3160.71	0.850
5p9p	$G^0(9p,p)$	367.50	fixed		459.38	0.800
5p9p	$G^2(9p,p)$	580.70	fixed		725.88	0.800
5p10p	E_{av}	521411.00	fixed		521411.00	1.000
5p10p	$\zeta(10p)$	13028.80	10	2	12333.10	1.056
5p10p	$\zeta(p)$	393.70	fixed		393.70	1.000
5p10p	$F^2(10p,p)$	1730.20	fixed		2035.53	0.850
5p10p	$G^0(10p,p)$	232.10	fixed		290.13	0.800
5p10p	$G^2(10p,p)$	371.60	fixed		464.50	0.800
5p4f	E_{av}	201858.50	fixed		201858.50	1.000
5p4f	$\zeta(4f)$	312.40	fixed		312.40	1.000
5p4f	$\zeta(5p)$	11624.80	9	2	11004.10	1.056
5p4f	$F^2(4f,5p)$	43435.80	fixed		51100.94	0.850
5p4f	$G^2(4f,5p)$	27627.30	fixed		34534.13	0.800
5p4f	$G^4(4f,5p)$	20453.90	fixed		25567.38	0.800
5p5f	E_{av}	368464.10	fixed		368464.10	1.000
5p5f	$\zeta(5p)$	12751.60	10	2	12070.70	1.056
5p5f	$\zeta(5f)$	81.20	fixed		81.20	1.000
5p5f	$F^2(5p,5f)$	18165.90	fixed		21371.65	0.850
5p5f	$G^2(5p,5f)$	4270.90	fixed		5338.63	0.800
5p5f	$G^4(5p,5f)$	3606.30	fixed		4507.88	0.800
5p6f	E_{av}	443747.40	fixed		443747.40	1.000
5p6f	$\zeta(5p)$	12907.80	10	2	12218.60	1.056
5p6f	$\zeta(6f)$	40.10	fixed		40.10	1.000
5p6f	$F^2(5p,6f)$	8507.80	fixed		10009.18	0.850
5p6f	$G^2(5p,6f)$	2567.10	fixed		3208.88	0.800
5p6f	$G^4(5p,6f)$	2066.50	fixed		2583.13	0.800
5p7f	E_{av}	485432.70	fixed		485432.70	1.000
5p7f	$\zeta(5p)$	12968.80	10	2	12276.30	1.056
5p7f	$\zeta(7f)$	23.10	fixed		23.10	1.000
5p7f	$F^2(5p,7f)$	4703.60	fixed		5533.65	0.850
5p7f	$G^2(5p,7f)$	1573.00	fixed		1966.25	0.800
5p7f	$G^4(5p,7f)$	1250.40	fixed		1563.00	0.800
5p8f	E_{av}	511097.80	fixed		511097.80	1.000
5p8f	$\zeta(5p)$	12998.00	10	2	12303.90	1.056
5p8f	$\zeta(8f)$	14.60	fixed		14.60	1.000
5p8f	$F^2(5p,8f)$	2887.50	fixed		3397.06	0.850
5p8f	$G^2(5p,8f)$	1018.10	fixed		1272.63	0.800
5p8f	$G^4(5p,8f)$	805.50	fixed		1006.88	0.800
5p9f	E_{av}	528022.70	fixed		528022.70	1.000

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p9f	$\zeta(5p)$	13013.70	10	2	12318.80	1.056
5p9f	$\zeta(9f)$	9.80	fixed		9.80	1.000
5p9f	$F^2(5p,9f)$	1905.40	fixed		2241.65	0.850
5p9f	$G^2(5p,9f)$	693.00	fixed		866.25	0.800
5p9f	$G^4(5p,9f)$	547.30	fixed		684.13	0.800
5p10f	E_{av}	539770.60	fixed		539770.60	1.000
5p10f	$\zeta(5p)$	13023.10	10	2	12327.70	1.056
5p10f	$\zeta(10f)$	6.90	fixed		6.90	1.000
5p10f	$F^2(5p,10f)$	1325.70	fixed		1559.65	0.850
5p10f	$G^2(5p,10f)$	492.00	fixed		615.00	0.800
5p10f	$G^4(5p,10f)$	388.10	fixed		485.13	0.800
$4f^2$	E_{av}	384129.20	fixed		384129.20	1.000
$4f^2$	$F^2(4f,4f)$	56513.40	fixed		66486.35	0.850
$4f^2$	$F^4(4f,4f)$	35065.70	fixed		41253.77	0.850
$4f^2$	$F^6(4f,4f)$	25114.20	fixed		29546.12	0.850
$4f^2$	$\alpha(4f)$	0.00	fixed		0.00	
$4f^2$	$\beta(4f)$	0.00	fixed		0.00	
$4f^2$	$G_a(4f)$	0.00	fixed		0.00	
$4f^2$	$\zeta(4f)$	279.60	fixed		279.60	1.000
$5d^2$	E_{av}	400448.80	fixed		400448.80	1.000
$5d^2$	$F^2(5d,5d)$	40350.20	fixed		47470.82	0.850
$5d^2$	$F^4(5d,5d)$	27593.20	fixed		32462.59	0.850
$5d^2$	$\alpha(5d)$	0.00	fixed		0.00	
$5d^2$	$\beta(5d)$	0.00	fixed		0.00	
$5d^2$	$T(5d)$	0.00	fixed		0.00	
$5d^2$	$\zeta(5d)$	868.90	fixed		868.90	1.000
$6s^2$	E_{av}	514101.60	fixed		514101.60	1.000
$6p^2$	E_{av}	609135.60	fixed		609135.60	1.000
$6p^2$	$F^2(6p,6p)$	26654.40	fixed		31358.12	0.850
$6p^2$	$\alpha(6p)$	0.00	fixed		0.00	
$6p^2$	$\zeta(6p)$	3888.60	fixed		3888.60	1.000
$5p^4$	E_{av}	310124.60	fixed		310124.60	1.000
$5p^4$	$F^2(5p,5p)$	49940.40	58	1	59870.94	0.834
$5p^4$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5p^4$	$\zeta(5p)$	11969.60	9	2	11330.50	1.056
$5s5p^26s$	E_{av}	387785.80	fixed		387785.80	1.000
$5s5p^26s$	$F^2(5p,5p)$	50763.20	59	1	60857.29	0.834
$5s5p^26s$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5s5p^26s$	$\zeta(5p)$	12656.30	10	2	11980.50	1.056
$5s5p^26s$	$G^1(6s,5p)$	63423.50	fixed		79279.38	0.800
$5s5p^26s$	$G^0(6s,s)$	3914.20	fixed		4892.75	0.800
$5s5p^26s$	$G^1(5p,s)$	5903.20	fixed		7379.00	0.800
$5s5p^27s$	E_{av}	518610.00	fixed		518610.00	1.000
$5s5p^27s$	$F^2(5p,5p)$	51163.00	59	1	61336.59	0.834
$5s5p^27s$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5s5p^27s$	$\zeta(5p)$	12842.60	10	2	12156.80	1.056
$5s5p^27s$	$G^1(7s,5p)$	63846.60	fixed		79808.25	0.800
$5s5p^27s$	$G^0(7s,s)$	1315.10	fixed		1643.88	0.800
$5s5p^27s$	$G^1(5p,s)$	1903.80	fixed		2379.75	0.800
$5s5p^28s$	E_{av}	582679.90	fixed		582679.90	1.000
$5s5p^28s$	$F^2(5p,5p)$	51256.90	59	1	61449.18	0.834
$5s5p^28s$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5s5p^28s$	$\zeta(5p)$	12897.40	10	2	12208.70	1.056
$5s5p^28s$	$G^1(8s,5p)$	63957.70	fixed		79947.13	0.800
$5s5p^28s$	$G^0(8s,s)$	625.50	fixed		781.88	0.800

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5s5p^{2}8s	$G^1(5p,s)$	902.40	fixed		1128.00	0.800
5s5p^{2}5d	E_{av}	332268.40	fixed		332268.40	1.000
5s5p^{2}5d	$F^2(5p,5p)$	50309.10	58	1	60312.94	0.834
5s5p^{2}5d	$\alpha(5p)$	-61.30	-6	3	0.00	
5s5p^{2}5d	$\zeta(5p)$	12285.10	9	2	11629.10	1.056
5s5p^{2}5d	$\zeta(5d)$	868.20	fixed		868.20	1.000
5s5p^{2}5d	$F^2(5p,5d)$	41905.10	fixed		49300.12	0.850
5s5p^{2}5d	$G^1(5s,5p)$	62904.40	fixed		78630.50	0.800
5s5p^{2}5d	$G^2(5s,5d)$	30895.30	fixed		38619.13	0.800
5s5p^{2}5d	$G^1(5p,5d)$	46326.30	fixed		57907.88	0.800
5s5p^{2}5d	$G^3(5p,5d)$	29445.10	fixed		36806.38	0.800
5s5p^{2}6d	E_{av}	499136.40	fixed		499136.40	1.000
5s5p^{2}6d	$F^2(5p,5p)$	51137.40	59	1	61305.88	0.834
5s5p^{2}6d	$\alpha(5p)$	-61.30	-6	3	0.00	
5s5p^{2}6d	$\zeta(5p)$	12803.80	10	2	12120.10	1.056
5s5p^{2}6d	$\zeta(6d)$	334.70	fixed		334.70	1.000
5s5p^{2}6d	$F^2(5p,6d)$	14552.20	fixed		17120.24	0.850
5s5p^{2}6d	$G^1(5s,5p)$	63826.90	fixed		79783.63	0.800
5s5p^{2}6d	$G^2(5s,6d)$	6662.00	fixed		8327.50	0.800
5s5p^{2}6d	$G^1(5p,6d)$	7361.80	fixed		9202.25	0.800
5s5p^{2}6d	$G^3(5p,6d)$	5520.40	fixed		6900.50	0.800
5s5p^{2}7d	E_{av}	573135.20	fixed		573135.20	1.000
5s5p^{2}7d	$F^2(5p,5p)$	51241.20	59	1	61430.35	0.834
5s5p^{2}7d	$\alpha(5p)$	-61.30	-6	3	0.00	
5s5p^{2}7d	$\zeta(5p)$	12882.70	10	2	12194.80	1.056
5s5p^{2}7d	$\zeta(7d)$	173.50	fixed		173.50	1.000
5s5p^{2}7d	$F^2(5p,7d)$	6844.00	fixed		8051.77	0.850
5s5p^{2}7d	$G^1(5s,5p)$	63948.90	fixed		79936.13	0.800
5s5p^{2}7d	$G^2(5s,7d)$	2832.30	fixed		3540.38	0.800
5s5p^{2}7d	$G^1(5p,7d)$	2895.00	fixed		3618.75	0.800
5s5p^{2}7d	$G^3(5p,7d)$	2295.60	fixed		2869.50	0.800
5s5p^{2}8d	E_{av}	613658.70	fixed		613658.70	1.000
5s5p^{2}8d	$F^2(5p,5p)$	51285.40	59	1	61483.41	0.834
5s5p^{2}8d	$\alpha(5p)$	-61.30	-6	3	0.00	
5s5p^{2}8d	$\zeta(5p)$	12913.40	10	2	12223.90	1.056
5s5p^{2}8d	$\zeta(8d)$	102.80	fixed		102.80	1.000
5s5p^{2}8d	$F^2(5p,8d)$	3812.10	fixed		4484.82	0.850
5s5p^{2}8d	$G^1(5s,5p)$	63999.00	fixed		79998.75	0.800
5s5p^{2}8d	$G^2(5s,8d)$	1521.70	fixed		1902.13	0.800
5s5p^{2}8d	$G^1(5p,8d)$	1501.30	fixed		1876.63	0.800
5s5p^{2}8d	$G^3(5p,8d)$	1224.10	fixed		1530.13	0.800
5p^{3}6p	E_{av}	580567.40	fixed		580567.40	1.000
5p^{3}6p	$F^2(5p,5p)$	51057.80	59	1	61210.47	0.834
5p^{3}6p	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}6p	$\zeta(5p)$	12730.70	10	2	12050.90	1.056
5p^{3}6p	$\zeta(6p)$	3556.70	fixed		3556.70	1.000
5p^{3}6p	$F^2(5p,6p)$	19512.30	fixed		22955.65	0.850
5p^{3}6p	$G^0(5p,6p)$	3622.60	fixed		4528.25	0.800
5p^{3}6p	$G^2(5p,6p)$	5124.70	fixed		6405.88	0.800
5p^{3}7p	E_{av}	688292.90	fixed		688292.90	1.000
5p^{3}7p	$F^2(5p,5p)$	51209.50	59	1	61392.35	0.834
5p^{3}7p	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}7p	$\zeta(5p)$	12804.30	10	2	12120.60	1.056
5p^{3}7p	$\zeta(7p)$	1718.80	fixed		1718.80	1.000
5p^{3}7p	$F^2(5p,7p)$	8636.80	fixed		10160.94	0.850

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p^{3}7p	$G^0(5p,7p)$	1269.40	fixed		1586.75	0.800
5p^{3}7p	$G^2(5p,7p)$	1957.70	fixed		2447.13	0.800
5p^{3}8p	E_{av}	743009.80	fixed		743009.80	1.000
5p^{3}8p	$F^2(5p,5p)$	51268.70	59	1	61463.29	0.834
5p^{3}8p	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}8p	$\zeta(5p)$	12834.40	10	2	12149.10	1.056
5p^{3}8p	$\zeta(8p)$	964.00	fixed		964.00	1.000
5p^{3}8p	$F^2(5p,8p)$	4551.00	fixed		5354.12	0.850
5p^{3}8p	$G^0(5p,8p)$	618.20	fixed		772.75	0.800
5p^{3}8p	$G^2(5p,8p)$	989.10	fixed		1236.38	0.800
5p^{3}9p	E_{av}	774986.90	fixed		774986.90	1.000
5p^{3}9p	$F^2(5p,5p)$	51296.20	59	1	61496.35	0.834
5p^{3}9p	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}9p	$\zeta(5p)$	12849.00	10	2	12162.90	1.056
5p^{3}9p	$\zeta(9p)$	596.90	fixed		596.90	1.000
5p^{3}9p	$F^2(5p,9p)$	2700.90	fixed		3177.53	0.850
5p^{3}9p	$G^0(5p,9p)$	354.40	fixed		443.00	0.800
5p^{3}9p	$G^2(5p,9p)$	578.30	fixed		722.88	0.800
5p^{3}10p	E_{av}	795374.50	fixed		795374.50	1.000
5p^{3}10p	$F^2(5p,5p)$	51311.20	60	1	61514.24	0.834
5p^{3}10p	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}10p	$\zeta(5p)$	12856.80	10	2	12170.30	1.056
5p^{3}10p	$\zeta(10p)$	395.40	fixed		395.40	1.000
5p^{3}10p	$F^2(5p,10p)$	1737.80	fixed		2044.47	0.850
5p^{3}10p	$G^0(5p,10p)$	224.00	fixed		280.00	0.800
5p^{3}10p	$G^2(5p,10p)$	369.80	fixed		462.25	0.800
5p^{3}4f	E_{av}	459512.10	fixed		459512.10	1.000
5p^{3}4f	$F^2(5p,5p)$	49232.00	57	1	59021.65	0.834
5p^{3}4f	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}4f	$\zeta(4f)$	329.60	fixed		329.60	1.000
5p^{3}4f	$\zeta(5p)$	11449.20	9	2	10837.80	1.056
5p^{3}4f	$F^2(4f,5p)$	43149.10	fixed		50763.65	0.850
5p^{3}4f	$G^2(4f,5p)$	26815.60	fixed		33519.50	0.800
5p^{3}4f	$G^4(4f,5p)$	19940.00	fixed		24925.00	0.800
5p^{3}5f	E_{av}	639346.20	fixed		639346.20	1.000
5p^{3}5f	$F^2(5p,5p)$	50879.50	59	1	60996.71	0.834
5p^{3}5f	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}5f	$\zeta(5p)$	12589.00	10	2	11916.80	1.056
5p^{3}5f	$\zeta(5f)$	81.20	fixed		81.20	1.000
5p^{3}5f	$F^2(5p,5f)$	18794.20	fixed		22110.82	0.850
5p^{3}5f	$G^2(5p,5f)$	4918.70	fixed		6148.38	0.800
5p^{3}5f	$G^4(5p,5f)$	4021.50	fixed		5026.88	0.800
5p^{3}6f	E_{av}	716416.10	fixed		716416.10	1.000
5p^{3}6f	$F^2(5p,5p)$	51137.80	59	1	61306.35	0.834
5p^{3}6f	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}6f	$\zeta(5p)$	12740.90	10	2	12060.60	1.056
5p^{3}6f	$\zeta(6f)$	40.20	fixed		40.20	1.000
5p^{3}6f	$F^2(5p,6f)$	8708.40	fixed		10245.18	0.850
5p^{3}6f	$G^2(5p,6f)$	2825.00	fixed		3531.25	0.800
5p^{3}6f	$G^4(5p,6f)$	2236.10	fixed		2795.13	0.800
5p^{3}7f	E_{av}	758772.60	fixed		758772.60	1.000
5p^{3}7f	$F^2(5p,5p)$	51230.60	59	1	61417.65	0.834
5p^{3}7f	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{3}7f	$\zeta(5p)$	12799.60	10	2	12116.10	1.056
5p^{3}7f	$\zeta(7f)$	23.10	fixed		23.10	1.000

Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
$5p^37f$	$F^2(5p,7f)$	4778.40	fixed		5621.65	0.850
$5p^37f$	$G^2(5p,7f)$	1688.10	fixed		2110.13	0.800
$5p^37f$	$G^4(5p,7f)$	1326.60	fixed		1658.25	0.800
$5p^38f$	E_{av}	784756.20	fixed		784756.20	1.000
$5p^38f$	$F^2(5p,5p)$	51272.80	59	1	61468.24	0.834
$5p^38f$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5p^38f$	$\zeta(5p)$	12827.30	10	2	12142.40	1.056
$5p^38f$	$\zeta(8f)$	14.60	fixed		14.60	1.000
$5p^38f$	$F^2(5p,8f)$	2922.30	fixed		3438.00	0.850
$5p^38f$	$G^2(5p,8f)$	1078.20	fixed		1347.75	0.800
$5p^38f$	$G^4(5p,8f)$	845.60	fixed		1057.00	0.800
$5p^39f$	E_{av}	801855.60	fixed		801855.60	1.000
$5p^39f$	$F^2(5p,5p)$	51295.50	59	1	61495.41	0.834
$5p^39f$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5p^39f$	$\zeta(5p)$	12842.50	10	2	12156.70	1.056
$5p^39f$	$\zeta(9f)$	9.80	fixed		9.80	1.000
$5p^39f$	$F^2(5p,9f)$	1923.60	fixed		2263.06	0.850
$5p^39f$	$G^2(5p,9f)$	728.10	fixed		910.13	0.800
$5p^39f$	$G^4(5p,9f)$	570.70	fixed		713.38	0.800
$5p^310f$	E_{av}	813709.00	fixed		813709.00	1.000
$5p^310f$	$F^2(5p,5p)$	51308.90	59	1	61511.53	0.834
$5p^310f$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5p^310f$	$\zeta(5p)$	12851.40	10	2	12165.20	1.056
$5p^310f$	$\zeta(10f)$	6.90	fixed		6.90	1.000
$5p^310f$	$F^2(5p,10f)$	1336.10	fixed		1571.88	0.850
$5p^310f$	$G^2(5p,10f)$	514.20	fixed		642.75	0.800
$5p^310f$	$G^4(5p,10f)$	403.00	fixed		503.75	0.800
5d6s	E_{av}	452690.10	fixed		452690.10	1.000
5d6s	$\zeta(5d)$	910.70	fixed		910.70	1.000
5d6s	$G^2(5d,6s)$	13699.00	fixed		17123.75	0.800
$5p^25d^2$	E_{av}	650290.10	fixed		650290.10	1.000
$5p^25d^2$	$F^2(5p,5p)$	50647.10	59	1	60718.12	0.834
$5p^25d^2$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5p^25d^2$	$F^2(5d,5d)$	40929.00	fixed		48151.77	0.850
$5p^25d^2$	$F^4(5d,5d)$	28007.90	fixed		32950.47	0.850
$5p^25d^2$	$\alpha(5d)$	0.00	fixed		0.00	
$5p^25d^2$	$\beta(5d)$	0.00	fixed		0.00	
$5p^25d^2$	$T(5d)$	0.00	fixed		0.00	
$5p^25d^2$	$\zeta(5p)$	12437.10	9	2	11773.00	1.056
$5p^25d^2$	$\zeta(5d)$	910.70	fixed		910.70	1.000
$5p^25d^2$	$F^2(5p,5d)$	42659.30	fixed		50187.41	0.850
$5p^25d^2$	$G^1(5p,5d)$	47420.90	fixed		59276.13	0.800
$5p^25d^2$	$G^3(5p,5d)$	30157.50	fixed		37696.88	0.800
$5p^25d6s$	E_{av}	710849.60	fixed		710849.60	1.000
$5p^25d6s$	$F^2(5p,5p)$	51098.80	59	1	61259.65	0.834
$5p^25d6s$	$\alpha(5p)$	-61.30	-6	3	0.00	
$5p^25d6s$	$\zeta(5p)$	12808.00	10	2	12124.10	1.056
$5p^25d6s$	$\zeta(5d)$	954.30	fixed		954.30	1.000
$5p^25d6s$	$F^2(5p,5d)$	43303.30	fixed		50945.06	0.850
$5p^25d6s$	$G^1(5p,5d)$	48198.70	fixed		60248.38	0.800
$5p^25d6s$	$G^3(5p,5d)$	30680.40	fixed		38350.50	0.800
$5p^25d6s$	$G^1(5p,6s)$	6003.00	fixed		7503.75	0.800
$5p^25d6s$	$G^2(5d,6s)$	12672.40	fixed		15840.50	0.800
$5p^26s^2$	E_{av}	780534.60	fixed		780534.60	1.000
$5p^26s^2$	$F^2(5p,5p)$	51550.30	60	1	61800.94	0.834

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p^{2}6s^2	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{2}6s^2	$\zeta(5p)$	13194.80	10	2	12490.20	1.056
5p^{2}4f^2	E_{av}	620435.50	fixed		620435.50	1.000
5p^{2}4f^2	$F^2(4f,4f)$	58660.50	fixed		69012.35	0.850
5p^{2}4f^2	$F^4(4f,4f)$	36480.00	fixed		42917.65	0.850
5p^{2}4f^2	$F^6(4f,4f)$	26150.00	fixed		30764.71	0.850
5p^{2}4f^2	$\alpha(4f)$	0.00	fixed		0.00	
5p^{2}4f^2	$\beta(4f)$	0.00	fixed		0.00	
5p^{2}4f^2	$G_a(4f)$	0.00	fixed		0.00	
5p^{2}4f^2	$F^2(5p,5p)$	48639.00	56	1	58310.71	0.834
5p^{2}4f^2	$\alpha(5p)$	-61.30	-6	3	0.00	
5p^{2}4f^2	$\zeta(4f)$	295.70	fixed		295.70	1.000
5p^{2}4f^2	$\zeta(5p)$	11028.30	8	2	10439.40	1.056
5p^{2}4f^2	$F^2(4f,5p)$	42997.20	fixed		50584.94	0.850
5p^{2}4f^2	$G^2(4f,5p)$	27988.40	fixed		34985.50	0.800
5p^{2}4f^2	$G^4(4f,5p)$	20576.60	fixed		25720.75	0.800
5s5p5d4f	E_{av}	489764.90	fixed		489764.90	1.000
5s5p5d4f	$\zeta(4f)$	333.00	fixed		333.00	1.000
5s5p5d4f	$\zeta(5p)$	11140.20	fixed		11140.20	1.000
5s5p5d4f	$\zeta(5d)$	812.20	fixed		812.20	1.000
5s5p5d4f	$F^2(4f,5p)$	43531.80	fixed		51213.88	0.850
5s5p5d4f	$F^2(4f,5d)$	30099.00	fixed		35410.59	0.850
5s5p5d4f	$F^4(4f,5d)$	16759.80	fixed		19717.41	0.850
5s5p5d4f	$F^2(5p,5d)$	41003.40	fixed		48239.29	0.850
5s5p5d4f	$G^3(4f,5s)$	28072.80	fixed		35091.00	0.800
5s5p5d4f	$G^2(4f,5p)$	26885.40	fixed		33606.75	0.800
5s5p5d4f	$G^4(4f,5p)$	20054.60	fixed		25068.25	0.800
5s5p5d4f	$G^1(4f,5d)$	17573.60	fixed		21967.00	0.800
5s5p5d4f	$G^3(4f,5d)$	13729.40	fixed		17161.75	0.800
5s5p5d4f	$G^5(4f,5d)$	10405.20	fixed		13006.50	0.800
5s5p5d4f	$G^1(5s,5p)$	62000.30	fixed		77500.38	0.800
5s5p5d4f	$G^2(5s,5d)$	29826.00	fixed		37282.50	0.800
5s5p5d4f	$G^1(5p,5d)$	45114.90	fixed		56393.63	0.800
5s5p5d4f	$G^3(5p,5d)$	28683.20	fixed		35854.00	0.800
5p6s	E_{av}	261854.90	82		262502.60	0.998
5p6s	$\zeta(5p)$	12815.20	68	1	12059.90	1.063
5p6s	$G^1(5p,6s)$	5512.50	400	2	7319.63	0.753
5p7s	E_{av}	393236.40	fixed		393236.40	1.000
5p7s	$\zeta(5p)$	13006.60	69	1	12240.00	1.063
5p7s	$G^1(5p,7s)$	1785.60	129	2	2371.00	0.753
5p8s	E_{av}	457209.10	fixed		457209.10	1.000
5p8s	$\zeta(5p)$	13062.80	70	1	12292.90	1.063
5p8s	$G^1(5p,8s)$	849.00	62	2	1127.25	0.753
5p9s	E_{av}	493662.60	fixed		493662.60	1.000
5p9s	$\zeta(5p)$	13086.80	70	1	12315.50	1.063
5p9s	$G^1(5p,9s)$	479.90	35	2	637.25	0.753
5p10s	E_{av}	516488.70	fixed		516488.70	1.000
5p10s	$\zeta(5p)$	13099.20	70	1	12327.10	1.063
5p10s	$G^1(5p,10s)$	300.10	22	2	398.50	0.753
5p5d	E_{av}	208717.90	95		210942.20	0.989
5p5d	$\zeta(5p)$	12445.20	66	1	11711.70	1.063
5p5d	$\zeta(5d)$	1145.70	72	8	847.20	1.352
5p5d	$F^2(5p,5d)$	38915.30	500	4	48875.77	0.796
5p5d	$G^1(5p,5d)$	41194.70	272	5	57132.38	0.721
5p5d	$G^3(5p,5d)$	26056.80	509	6	36310.50	0.718
5p6d	E_{av}	374595.20	fixed		374595.20	1.000

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p6d	$\zeta(5p)$	12966.40	69	1	12202.20	1.063
5p6d	$\zeta(6d)$	450.90	28	8	333.40	1.352
5p6d	$F^2(5p,6d)$	13597.30	175	4	17077.53	0.796
5p6d	$G^1(5p,6d)$	6769.70	45	5	9388.88	0.721
5p6d	$G^3(5p,6d)$	5019.50	98	6	6994.75	0.718
5p7d	E_{av}	448002.60	fixed		448002.60	1.000
5p7d	$\zeta(5p)$	13047.00	70	1	12278.00	1.063
5p7d	$\zeta(7d)$	234.20	15	8	173.20	1.352
5p7d	$F^2(5p,7d)$	6403.90	82	4	8042.94	0.796
5p7d	$G^1(5p,7d)$	2665.40	18	5	3696.63	0.721
5p7d	$G^3(5p,7d)$	2088.40	41	6	2910.25	0.718
5p8d	E_{av}	488324.00	fixed		488324.00	1.000
5p8d	$\zeta(5p)$	13078.40	70	1	12307.60	1.063
5p8d	$\zeta(8d)$	138.90	9	8	102.70	1.352
5p8d	$F^2(5p,8d)$	3569.60	46	4	4483.29	0.796
5p8d	$G^1(5p,8d)$	1382.10	9	5	1916.88	0.721
5p8d	$G^3(5p,8d)$	1113.40	22	6	1551.50	0.718
5p9d	E_{av}	513098.50	fixed		513098.50	1.000
5p9d	$\zeta(5p)$	13094.30	70	1	12322.50	1.063
5p9d	$\zeta(9d)$	89.40	6	8	66.10	1.352
5p9d	$F^2(5p,9d)$	2205.50	28	4	2770.00	0.796
5p9d	$G^1(5p,9d)$	823.00	5	5	1141.38	0.721
5p9d	$G^3(5p,9d)$	673.70	13	6	938.88	0.718
5p10d	E_{av}	529448.70	fixed		529448.70	1.000
5p10d	$\zeta(5p)$	13103.30	70	1	12331.00	1.063
5p10d	$\zeta(10d)$	61.00	4	8	45.10	1.353
5p10d	$F^2(5p,10d)$	1462.90	19	4	1837.29	0.796
5p10d	$G^1(5p,10d)$	534.40	4	5	741.13	0.721
5p10d	$G^3(5p,10d)$	442.00	9	6	616.00	0.718
5s5p^3	E_{av}	158786.20	108		158557.30	1.001
5s5p^3	$F^2(5p,5p)$	50863.20	408	3	59873.53	0.850
5s5p^3	$\alpha(5p)$	-81.50	-36	9	0.00	
5s5p^3	$\zeta(5p)$	12109.70	65	1	11396.00	1.063
5s5p^3	$G^1(5s,5p)$	57837.70	167	7	78111.88	0.740
5s5p^{2}6p	E_{av}	433183.30	fixed		433183.30	1.000
5s5p^{2}6p	$F^2(5p,5p)$	52014.40	417	3	61228.71	0.850
5s5p^{2}6p	$\alpha(5p)$	-81.50	-36	9	0.00	
5s5p^{2}6p	$\zeta(5p)$	12889.80	69	1	12130.10	1.063
5s5p^{2}6p	$\zeta(6p)$	3539.40	fixed		3539.40	1.000
5s5p^{2}6p	$F^2(5p,6p)$	19386.70	fixed		22807.88	0.850
5s5p^{2}6p	$G^1(5s,5p)$	59036.50	171	7	79730.88	0.740
5s5p^{2}6p	$G^1(5s,6p)$	5993.30	fixed		7491.63	0.800
5s5p^{2}6p	$G^0(5p,6p)$	3700.10	fixed		4625.13	0.800
5s5p^{2}6p	$G^2(5p,6p)$	5112.80	fixed		6391.00	0.800
5s5p^{2}7p	E_{av}	540226.80	fixed		540226.80	1.000
5s5p^{2}7p	$F^2(5p,5p)$	52161.50	418	3	61401.88	0.850
5s5p^{2}7p	$\alpha(5p)$	-81.50	-36	9	0.00	
5s5p^{2}7p	$\zeta(5p)$	12962.00	69	1	12198.00	1.063
5s5p^{2}7p	$\zeta(7p)$	1710.70	fixed		1710.70	1.000
5s5p^{2}7p	$F^2(5p,7p)$	8593.70	fixed		10110.24	0.850
5s5p^{2}7p	$G^1(5s,5p)$	59171.80	171	7	79913.63	0.740
5s5p^{2}7p	$G^1(5s,7p)$	2237.30	fixed		2796.63	0.800
5s5p^{2}7p	$G^0(5p,7p)$	1292.30	fixed		1615.38	0.800
5s5p^{2}7p	$G^2(5p,7p)$	1957.00	fixed		2446.25	0.800

Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
$5s5p^28p$	E_{av}	594697.10	fixed		594697.10	1.000
$5s5p^28p$	$F^2(5p,5p)$	52221.70	419	3	61472.71	0.850
$5s5p^28p$	$\alpha(5p)$	-81.50	-36	9	0.00	
$5s5p^28p$	$\zeta(5p)$	12992.50	69	1	12226.70	1.063
$5s5p^28p$	$\zeta(8p)$	960.50	fixed		960.50	1.000
$5s5p^28p$	$F^2(5p,8p)$	4534.80	fixed		5335.06	0.850
$5s5p^28p$	$G^1(5s,5p)$	59228.90	171	7	79990.75	0.740
$5s5p^28p$	$G^1(5s,8p)$	1118.30	fixed		1397.88	0.800
$5s5p^28p$	$G^0(5p,8p)$	629.10	fixed		786.38	0.800
$5s5p^28p$	$G^2(5p,8p)$	990.10	fixed		1237.63	0.800
$5s5p^24f$	E_{av}	319549.20	fixed		319549.20	1.000
$5s5p^24f$	$F^2(5p,5p)$	50163.10	402	3	59049.41	0.850
$5s5p^24f$	$\alpha(5p)$	-81.50	-36	9	0.00	
$5s5p^24f$	$\zeta(4f)$	320.80	fixed		320.80	1.000
$5s5p^24f$	$\zeta(5p)$	11601.30	62	1	10917.50	1.063
$5s5p^24f$	$F^2(4f,5p)$	43297.90	fixed		50938.71	0.850
$5s5p^24f$	$G^3(4f,5s)$	28181.50	fixed		35226.88	0.800
$5s5p^24f$	$G^2(4f,5p)$	27235.30	fixed		34044.13	0.800
$5s5p^24f$	$G^4(4f,5p)$	20205.70	fixed		25257.13	0.800
$5s5p^24f$	$G^1(5s,5p)$	57009.20	165	7	76992.88	0.740
$5s5p^25f$	E_{av}	492447.80	fixed		492447.80	1.000
$5s5p^25f$	$F^2(5p,5p)$	51824.00	416	3	61004.59	0.850
$5s5p^25f$	$\alpha(5p)$	-81.50	-36	9	0.00	
$5s5p^25f$	$\zeta(5p)$	12741.80	68	1	11990.80	1.063
$5s5p^25f$	$\zeta(5f)$	81.10	fixed		81.10	1.000
$5s5p^25f$	$F^2(5p,5f)$	18460.40	fixed		21718.12	0.850
$5s5p^25f$	$G^1(5s,5p)$	58818.50	170	7	79436.38	0.740
$5s5p^25f$	$G^3(5s,5f)$	2828.60	fixed		3535.75	0.800
$5s5p^25f$	$G^2(5p,5f)$	4572.30	fixed		5715.38	0.800
$5s5p^25f$	$G^4(5p,5f)$	3798.70	fixed		4748.38	0.800
$5s5p^26f$	E_{av}	568603.40	fixed		568603.40	1.000
$5s5p^26f$	$F^2(5p,5p)$	52086.20	418	3	61313.18	0.850
$5s5p^26f$	$\alpha(5p)$	-81.50	-36	9	0.00	
$5s5p^26f$	$\zeta(5p)$	12136.40	fixed		12136.40	1.000
$5s5p^26f$	$\zeta(6f)$	40.10	fixed		40.10	1.000
$5s5p^26f$	$F^2(5p,6f)$	8604.40	fixed		10122.82	0.850
$5s5p^26f$	$G^1(5s,5p)$	59082.40	171	7	79792.88	0.740
$5s5p^26f$	$G^3(5s,6f)$	1647.60	fixed		2059.50	0.800
$5s5p^26f$	$G^2(5p,6f)$	2691.40	fixed		3364.25	0.800
$5s5p^26f$	$G^4(5p,6f)$	2148.10	fixed		2685.13	0.800
$5s5p^27f$	E_{av}	610614.10	fixed		610614.10	1.000
$5s5p^27f$	$F^2(5p,5p)$	52182.00	419	3	61426.00	0.850
$5s5p^27f$	$\alpha(5p)$	-81.50	-36	9	0.00	
$5s5p^27f$	$\zeta(5p)$	12956.60	69	1	12192.90	1.063
$5s5p^27f$	$\zeta(7f)$	23.10	fixed		23.10	1.000
$5s5p^27f$	$F^2(5p,7f)$	4739.30	fixed		5575.65	0.850
$5s5p^27f$	$G^1(5s,5p)$	59181.30	171	7	79926.38	0.740
$5s5p^27f$	$G^3(5s,7f)$	1031.00	fixed		1288.75	0.800
$5s5p^27f$	$G^2(5p,7f)$	1629.20	fixed		2036.50	0.800
$5s5p^27f$	$G^4(5p,7f)$	1287.50	fixed		1609.38	0.800
$5s5p^28f$	E_{av}	636434.50	fixed		636434.50	1.000
$5s5p^28f$	$F^2(5p,5p)$	52225.70	419	3	61477.41	0.850
$5s5p^28f$	$\alpha(5p)$	-81.50	-36	9	0.00	
$5s5p^28f$	$\zeta(5p)$	12984.90	69	1	12219.60	1.063
$5s5p^28f$	$\zeta(8f)$	14.60	fixed		14.60	1.000

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5s5p^{2}8f	$F^2(5p,8f)$	2904.50	fixed		3417.06	0.850
5s5p^{2}8f	$G^1(5s,5p)$	59226.90	171	7	79988.00	0.740
5s5p^{2}8f	$G^3(5s,8f)$	679.90	fixed		849.88	0.800
5s5p^{2}8f	$G^2(5p,8f)$	1047.70	fixed		1309.63	0.800
5s5p^{2}8f	$G^4(5p,8f)$	825.20	fixed		1031.50	0.800
5p^{3}6s	E_{av}	536194.20	fixed		536194.20	1.000
5p^{3}6s	$F^2(5p,5p)$	51696.90	415	3	60854.94	0.850
5p^{3}6s	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}6s	$\zeta(5p)$	12653.30	68	1	11907.50	1.063
5p^{3}6s	$G^1(5p,6s)$	5618.90	407	2	7460.88	0.753
5p^{3}7s	E_{av}	667005.40	fixed		667005.40	1.000
5p^{3}7s	$F^2(5p,5p)$	52099.20	418	3	61328.47	0.850
5p^{3}7s	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}7s	$\zeta(5p)$	12836.90	69	1	12080.30	1.063
5p^{3}7s	$G^1(5p,7s)$	1912.60	fixed		2390.75	0.800
5p^{3}8s	E_{av}	731155.30	fixed		731155.30	1.000
5p^{3}8s	$F^2(5p,5p)$	52194.00	419	3	61440.12	0.850
5p^{3}8s	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}8s	$\zeta(5p)$	12891.20	69	1	12131.40	1.063
5p^{3}8s	$G^1(5p,8s)$	903.40	fixed		1129.25	0.800
5p^{3}9s	E_{av}	767693.80	fixed		767693.80	1.000
5p^{3}9s	$F^2(5p,5p)$	52232.30	419	3	61485.18	0.850
5p^{3}9s	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}9s	$\zeta(5p)$	12914.50	69	1	12153.30	1.063
5p^{3}9s	$G^1(5p,9s)$	509.10	fixed		636.38	0.800
5p^{3}10s	E_{av}	790568.10	fixed		790568.10	1.000
5p^{3}10s	$F^2(5p,5p)$	52251.70	419	3	61508.00	0.850
5p^{3}10s	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}10s	$\zeta(5p)$	12926.50	69	1	12164.60	1.063
5p^{3}10s	$G^1(5p,10s)$	317.90	fixed		397.38	0.800
5p^{3}5d	E_{av}	476284.60	fixed		476284.60	1.000
5p^{3}5d	$F^2(5p,5p)$	51224.20	411	3	60298.47	0.850
5p^{3}5d	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}5d	$\zeta(5p)$	12276.50	66	1	11552.90	1.063
5p^{3}5d	$\zeta(5d)$	1204.20	75	8	890.50	1.352
5p^{3}5d	$F^2(5p,5d)$	39602.70	509	4	49739.06	0.796
5p^{3}5d	$G^1(5p,5d)$	42328.30	280	5	58704.63	0.721
5p^{3}5d	$G^3(5p,5d)$	26778.50	523	6	37316.25	0.718
5p^{3}6d	E_{av}	646655.70	fixed		646655.70	1.000
5p^{3}6d	$F^2(5p,5p)$	52073.50	418	3	61298.24	0.850
5p^{3}6d	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}6d	$\zeta(5p)$	12799.30	68	1	12044.90	1.063
5p^{3}6d	$\zeta(6d)$	454.40	28	8	336.00	1.352
5p^{3}6d	$F^2(5p,6d)$	14588.50	fixed		17162.94	0.850
5p^{3}6d	$G^1(5p,6d)$	7204.60	fixed		9005.75	0.800
5p^{3}6d	$G^3(5p,6d)$	5440.40	fixed		6800.50	0.800
5p^{3}7d	E_{av}	721253.90	fixed		721253.90	1.000
5p^{3}7d	$F^2(5p,5p)$	52179.10	419	3	61422.59	0.850
5p^{3}7d	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}7d	$\zeta(5p)$	12877.30	69	1	12118.30	1.063
5p^{3}7d	$\zeta(7d)$	235.20	15	8	173.90	1.353
5p^{3}7d	$F^2(5p,7d)$	6853.10	fixed		8062.47	0.850
5p^{3}7d	$G^1(5p,7d)$	2832.40	fixed		3540.50	0.800
5p^{3}7d	$G^3(5p,7d)$	2263.10	fixed		2828.88	0.800
5p^{3}8d	E_{av}	761986.60	fixed		761986.60	1.000

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5p^{3}8d	$F^2(5p,5p)$	52223.70	419	3	61475.06	0.850
5p^{3}8d	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}8d	$\zeta(5p)$	12907.70	69	1	12146.90	1.063
5p^{3}8d	$\zeta(8d)$	139.40	9	8	103.10	1.352
5p^{3}8d	$F^2(5p,8d)$	3814.40	fixed		4487.53	0.850
5p^{3}8d	$G^1(5p,8d)$	1469.50	fixed		1836.88	0.800
5p^{3}8d	$G^3(5p,8d)$	1207.30	fixed		1509.13	0.800
5p^{3}9d	E_{av}	786954.90	fixed		786954.90	1.000
5p^{3}9d	$F^2(5p,5p)$	52246.70	419	3	61502.12	0.850
5p^{3}9d	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}9d	$\zeta(5p)$	12922.70	69	1	12161.00	1.063
5p^{3}9d	$\zeta(9d)$	89.70	6	8	66.30	1.353
5p^{3}9d	$F^2(5p,9d)$	2354.60	fixed		2770.12	0.850
5p^{3}9d	$G^1(5p,9d)$	875.70	fixed		1094.63	0.800
5p^{3}9d	$G^3(5p,9d)$	731.20	fixed		914.00	0.800
5p^{3}10d	E_{av}	803412.10	fixed		803412.10	1.000
5p^{3}10d	$F^2(5p,5p)$	52259.70	419	3	61517.41	0.850
5p^{3}10d	$\alpha(5p)$	-81.50	-36	9	0.00	
5p^{3}10d	$\zeta(5p)$	12931.10	69	1	12168.90	1.063
5p^{3}10d	$\zeta(10d)$	61.10	4	8	45.20	1.352
5p^{3}10d	$F^2(5p,10d)$	1560.20	fixed		1835.53	0.850
5p^{3}10d	$G^1(5p,10d)$	568.40	fixed		710.50	0.800
5p^{3}10d	$G^3(5p,10d)$	479.60	fixed		599.50	0.800
5s5p5d^2	E_{av}	513986.70	fixed		513986.70	1.000
5s5p5d^2	$F^2(5d,5d)$	40631.80	fixed		47802.12	0.850
5s5p5d^2	$F^4(5d,5d)$	27794.90	fixed		32699.88	0.850
5s5p5d^2	$\alpha(5d)$	0.00	fixed		0.00	
5s5p5d^2	$\beta(5d)$	0.00	fixed		0.00	
5s5p5d^2	$T(5d)$	0.00	fixed		0.00	
5s5p5d^2	$\zeta(5p)$	12602.60	67	1	11859.80	1.063
5s5p5d^2	$\zeta(5d)$	1202.30	75	8	889.10	1.352
5s5p5d^2	$F^2(5p,5d)$	39627.40	509	4	49770.12	0.796
5s5p5d^2	$G^1(5s,5p)$	58598.50	170	7	79139.25	0.740
5s5p5d^2	$G^2(5s,5d)$	31283.80	fixed		39104.75	0.800
5s5p5d^2	$G^1(5p,5d)$	42188.20	279	5	58510.25	0.721
5s5p5d^2	$G^3(5p,5d)$	26699.70	522	6	37206.38	0.718
5s5p5d6s	E_{av}	570183.00	fixed		570183.00	1.000
5s5p5d6s	$\zeta(5p)$	12972.30	69	1	12207.70	1.063
5s5p5d6s	$\zeta(5d)$	1260.20	79	8	931.90	1.352
5s5p5d6s	$F^2(5p,5d)$	40230.70	517	4	50527.88	0.796
5s5p5d6s	$G^1(6s,5p)$	59065.50	171	7	79770.00	0.740
5s5p5d6s	$G^2(6s,5d)$	31715.30	fixed		39644.13	0.800
5s5p5d6s	$G^0(6s,s)$	3958.50	fixed		4948.13	0.800
5s5p5d6s	$G^1(5p,5d)$	42892.70	284	5	59487.38	0.721
5s5p5d6s	$G^3(5p,5d)$	27170.00	531	6	37861.75	0.718
5s5p5d6s	$G^1(5p,s)$	5938.40	fixed		7423.00	0.800
5s5p5d6s	$G^2(5d,s)$	13219.70	fixed		16524.63	0.800
5s5p6s^2	E_{av}	635459.70	fixed		635459.70	1.000
5s5p6s^2	$\zeta(5p)$	13358.10	71	1	12570.80	1.063
5s5p6s^2	$G^1(5s,5p)$	59529.50	172	7	80396.63	0.740
5s5p4f^2	E_{av}	491309.90	fixed		491309.90	1.000
5s5p4f^2	$F^2(4f,4f)$	57554.90	fixed		67711.65	0.850
5s5p4f^2	$F^4(4f,4f)$	35751.00	fixed		42060.00	0.850
5s5p4f^2	$F^6(4f,4f)$	25615.80	fixed		30136.24	0.850
5s5p4f^2	$\alpha(4f)$	0.00	fixed		0.00	

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Table A1. *Cont.*

Configuration[a]	Parameter[a]	LSF [a] (cm^{-1})	Unc[b] (cm^{-1})	Index [c]	HFR [a] (cm^{-1})	LSF/HFR[a]
5s5p4f^2	$\beta(4f)$	0.00	fixed		0.00	
5s5p4f^2	$G_a(4f)$	0.00	fixed		0.00	
5s5p4f^2	$\zeta(4f)$	287.30	fixed		287.30	1.000
5s5p4f^2	$\zeta(5p)$	11196.10	60	1	10536.20	1.063
5s5p4f^2	$F^2(4f,5p)$	43131.40	fixed		50742.82	0.850
5s5p4f^2	$G^3(4f,5s)$	28729.60	fixed		35912.00	0.800
5s5p4f^2	$G^2(4f,5p)$	28380.30	fixed		35475.38	0.800
5s5p4f^2	$G^4(4f,5p)$	20822.80	fixed		26028.50	0.800
5s5p4f^2	$G^1(5s,5p)$	56322.50	163	7	76065.50	0.740
5p6s-5p5d	$R_d^2(5p,6s,5p,5d)^d$	-9894.80	-77	10	-13324.40	0.743
5p6s-5p5d	$R_e^1(5p,6s,5p,5d)$	-3800.60	-29	10	-5117.90	0.743
5p6s-5s5p^3	$R_d^1(5s,6s,5p,5p)$	-662.90	-5	10	-892.70	0.743
5p5d-5s5p^3	$R_d^1(5s,5d,5p,5p)$	48226.90	373	10	64942.70	0.743

[a] Configurations involved in the calculations and their Slater parameters with the corresponding Hartree–Fock (HFR) and/or least-squares-fitted (LSF) values and their ratios. [b] Uncertainty of each parameter represents its standard deviation. [c] Parameters in each numbered group were linked together with their ratio fixed at the HFR level. [d] All other configuration-interaction (R^k) parameters for both parities were fixed at 70% of their HFR values.

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