

$5s^25p^2(5d + 6s)$ configurations in triply ionized xenon (Xe IV)

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The spectrum of triply ionized xenon (Xe IV) has been observed in the region 570–6900 Å. The configurations $5s^25p^25d$ and $5s^25p^26s$ have been studied and the energy levels reported for these configurations by Moore [*Atomic Energy Levels*, Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1971)] were revised and extended to include seven new levels. The configuration $5s5p^4$ was included in the analysis to take into account the strong interaction between this configuration and $5s^25p^25d$. Configuration-interaction Rydberg series have been also included in the calculations. This investigation was supported by Hartree-Fock calculations.

INTRODUCTION

The triply ionized xenon atom is isoelectronic with neutral antimony. The ground-state configuration is $5s^25p^3$ and the lowest excited configuration is $5s5p^4$. The spectrum of Xe IV was studied by Boyce and Humphreys and the results were published in *Atomic Energy Levels*¹ (AEL). Subsequently, Di Rocco *et al.*² published the results of the analysis of the ground-state configuration and the first excited-state configuration.

There is great interest in spectroscopy data from xenon due to applications in collision physics and laser physics. In the present investigation we have photographically recorded xenon spectra in the 240–6900-Å range. When analyzing the experimental data we have made use of Hartree-Fock calculations and parametric fits. Configuration-interaction (CI) effects, including Rydberg-series CI, have been included in the calculations. The present work concerns the study of the configurations $5s^25p^25d$ and $5s^25p^26s$.

EXPERIMENTAL METHODS

In the vacuum ultraviolet region we have used three different light sources: a direct-current hollow cathode discharge,³ a θ -pinch discharge,⁴ and a capillary pulsed discharge.⁵ The first two light sources, built at the Lund Institute of Technology, Sweden, and a 3-m normal incidence spectrograph, built at Lund, were used to record the spectra. This spectrograph is equipped with a ruled grating having 1200 lines/mm. The plate factor in the first diffraction order is 2.77 Å/mm. The spectra were exposed on Kodak standing-wave radio plates, and lines from C, N, and O were used as internal standards.

The capillary pulsed discharge source was built at the Centro de Investigaciones Opticas, Argentina, and a 3-m normal incidence spectrograph (Hilger & Watts) was used to record the spectra. This spectrograph is equipped with a ruled grating having 1200 lines/mm. The plate factor in the first diffraction order is 2.77 Å/mm. Ilford Q-2 plates were used to record the spectra. Known lines of C, N, and O were used as internal standards.

In the 2500–6900-Å range the spectrum was obtained using two different laser-tube-like sources. One of them is 1 m in length and has a 3-mm inner diameter,⁶ and the other is 20 cm long and has a 3-mm inner diameter.⁷ Both tubes were viewed end on. To record the spectra, the 3.4 m Ebert plane-grating spectrograph at Centro de Investigaciones Opticas was used. The grating has 600 lines/mm, corresponding to a plate factor of 5 Å/mm in the first diffraction order. Kodak 103 a-O and Kodak 103 a-F plates were used to record the spectra in the first, second, the third diffraction orders.

The $5s^25p^3-5s^25p^25d$ and $5s^25p^3-5s^25p^26s$ combinations observed in the present work are listed in Table I. The wavelength values are estimated to be correct to ± 0.01 Å and the intensities of the lines are based on visual estimates.

ANALYSIS

We present in Table II the values of the energy levels experimentally established in the present work. Seven of them are new and the rest correspond to undesignated levels from Boyce and Humphreys.¹ The levels were determined from combinations with levels of the ground-state configuration and also from combinations with higher-lying odd levels tentatively assigned to the

TABLE I. Classified 5s²5p³-5s²5p²5d, 6s lines in the Xe IV spectrum.

Intensity	λ_{vac} (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc. ^b	
0.5	558.65	179 003.0	2.1	⁴ S _{3/2} -(¹ D)5d ² D _{5/2}
-1 ^a	577.295 ^a	173 221.7	2.0	⁴ S _{3/2} -(³ P)6s ² P _{3/2}
10	578.40	172 890.7	2.4	⁴ S _{3/2} -(¹ D)5d ² P _{1/2}
2	578.76	172 783.2	2.3	² D _{3/2} -(¹ D)5d ² D _{3/2}
2	586.54	170 491.4	0.0	⁴ S _{3/2} -(¹ D)5d ² P _{3/2}
6	587.77	170 134.6	2.6	⁴ S _{3/2} -(³ P)6s ⁴ P _{5/2}
4	591.70	169 004.6	1.8	⁴ S _{3/2} -(³ P)5d ² D _{5/2}
3	593.34	168 537.4	8.2	² D _{5/2} -(¹ D)5d ² D _{3/2}
1	598.06	167 207.3	6.9	⁴ S _{3/2} -(³ P)6s ² P _{1/2}
8	603.38	165 733.0	4.1	² D _{3/2} -(¹ D)5d ² D _{5/2}
11	605.03	165 281.1	0.5	⁴ S _{3/2} -(³ P)6s ⁴ P _{3/2}
2	611.27	163 593.8	6.2	⁴ S _{3/2} -(³ P)5d ² D _{3/2}
6 ^a	619.238 ^a	161 488.8	90.0	² D _{5/2} -(¹ D)5d ² D _{5/2}
8	619.45	161 433.5	4.1	⁴ S _{3/2} -(³ P)5d ⁴ P _{3/2}
4	625.17	159 956.5	4.0	² D _{3/2} -(³ P)6s ² P _{3/2}
10	626.40	159 642.4	3.1	⁴ S _{3/2} -(³ P)5d ⁴ P _{5/2}
7	626.47	159 624.6	4.4	² D _{3/2} -(¹ D)5d ² P _{1/2}
7	636.05	157 220.3	2.0	² D _{3/2} -(¹ D)5d ² P _{3/2}
6	637.50	156 862.7	4.6	² D _{3/2} -(³ P)6s ⁴ P _{5/2}
11	642.12	155 734.1	3.8	² D _{3/2} -(³ P)5d ² D _{5/2}
11	642.22	155 709.9	9.9	² D _{5/2} -(³ P)6s ² P _{3/2}
5	647.11	154 533.2	2.0	⁴ S _{3/2} -(³ P)6s ⁴ P _{1/2}
6	649.61	153 938.5	8.9	² D _{3/2} -(³ P)6s ² P _{1/2}
6	653.69	152 977.7	7.9	² D _{5/2} -(¹ D)5d ² P _{3/2}
6	655.22	152 620.5	0.5	² D _{5/2} -(³ P)6s ⁴ P _{5/2}
0.5	657.83	152 015.0	2.5	² D _{3/2} -(³ P)6s ⁴ P _{3/2}
4	660.12	151 487.6	9.7	² D _{5/2} -(³ P)5d ² D _{5/2}
8	665.21	150 328.5	8.2	² D _{3/2} -(³ P)5d ² D _{3/2}
11	672.56	148 685.6	5.2	⁴ S _{3/2} -(³ P)5d ⁴ D _{3/2}
2 ^a	674.919 ^a	148 165.9	6.1	² D _{3/2} -(³ P)5d ⁴ P _{3/2}
4	676.74	147 767.2	8.4	² D _{5/2} -(³ P)6s ⁴ P _{3/2}
4	683.17	146 376.5	5.1	² D _{3/2} -(³ P)5d ⁴ P _{5/2}
9	683.97	146 205.2	6.4	⁴ S _{3/2} -(³ P)5d ⁴ D _{3/2}
7	684.54	146 083.5	4.1	⁴ D _{5/2} -(³ P)5d ² D _{3/2}
0.5	688.78	145 184.2	6.0	² P _{1/2} -(³ P)6s ² P _{3/2}
0 ^a	689.147 ^a	145 106.9	5.7	⁴ S _{3/2} -(³ P)5d ⁴ D _{1/2}
4	690.33	144 858.3	6.4	² P _{1/2} -(¹ D)5d ² P _{1/2}
7	697.58	143 352.7	1.7	² P _{3/2} -(¹ D)5d ² D _{5/2}
5	703.57	142 132.3	1.0	² D _{5/2} -(³ P)5d ⁴ P _{5/2}
12	705.09	141 825.9	4.4	⁴ S _{3/2} -(¹ D)5d ² F _{5/2}
8	707.90	141 262.9	4.0	² D _{3/2} -(³ P)6s ⁴ P _{1/2}
8	718.54	139 171.1	0.9	² P _{1/2} -(³ P)6s ² P _{1/2}
11	722.80	138 350.9	1.8	² D _{5/2} -(³ P)5d ² F _{7/2}
4 ^a	728.634 ^a	137 243.1	4.5	² P _{1/2} -(³ P)6s ⁴ P _{3/2}
12	732.63	136 494.5	5.7	⁴ S _{3/2} -(³ P)5d ⁴ F _{5/2}
4	737.67	135 562.0	0.2	² P _{1/2} -(³ P)5d ² D _{3/2}
1	738.46	135 416.9	7.2	² D _{3/2} -(³ P)5d ⁴ D _{5/2}
11	740.85	134 980.1	0.6	⁴ S _{3/2} -(³ P)5d ⁴ F _{3/2}

TABLE I. (Continued).

Intensity	λ_{vac} (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc. ^b	
0 ^a	741.621 ^a	134 839.8	39.6	$^2P_{3/2}-(^1D)5d\ ^2P_{3/2}$
4	749.64	133 397.4	8.1	$^2P_{1/2}-(^3P)5d\ ^4P_{3/2}$
5	751.73	133 026.5	7.1	$^4S_{3/2}-(^3P)5d\ ^2P_{3/2}$
3	752.23	132 938.1	8.4	$^2D_{3/2}-(^3P)5d\ ^4D_{3/2}$
8	758.51	131 837.4	7.7	$^2D_{3/2}-(^3P)5d\ ^4D_{1/2}$
2	762.35	131 173.3	3.1	$^2D_{5/2}-(^3P)5d\ ^4D_{5/2}$
3	777.04	128 693.5	4.3	$^2D_{5/2}-(^3P)5d\ ^4D_{3/2}$
6	777.88	128 554.5	6.4	$^2D_{3/2}-(^1D)5d\ ^2F_{5/2}$
6	781.58	127 946.0	5.8	$^2P_{3/2}-(^3P)5d\ ^2D_{3/2}$
11	784.32	127 499.0	9.2	$^2D_{5/2}-(^3P)5d\ ^4D_{7/2}$
11	805.71	124 114.1	3.0	$^2D_{5/2}-(^3P)5d\ ^4F_{7/2}$
2	811.50	123 228.6	7.7	$^2D_{3/2}-(^3P)5d\ ^4F_{5/2}$
2	821.60	121 713.7	2.6	$^2D_{3/2}-(^3P)5d\ ^4F_{3/2}$
7	835.01	119 759.0	9.1	$^2D_{3/2}-(^3P)5d\ ^2P_{3/2}$
6	840.44	118 985.3	3.6	$^2D_{5/2}-(^3P)5d\ ^4F_{5/2}$
0.5	846.23	118 171.2	0.4	$^2P_{1/2}-(^3P)5d\ ^4D_{3/2}$
10	851.29	117 468.8	8.5	$^2D_{5/2}-(^3P)5d\ ^4F_{3/2}$
6	854.19	117 070.0	69.7	$^2P_{1/2}-(^3P)5d\ ^4D_{1/2}$
6	865.68	115 516.1	5.0	$^2D_{5/2}-(^3P)5d\ ^2P_{3/2}$
8	904.51	110 557.1	6.0	$^2P_{3/2}-(^3P)5d\ ^4D_{3/2}$
4	952.47	104 990.2	1.1	$^2P_{1/2}-(^3P)5d\ ^2P_{3/2}$
11	1006.75	99 329.5	30.2	$^2P_{3/2}-(^3P)5d\ ^4F_{3/2}$
1 ^a	1026.935 ^a	97 377.1	6.7	$^2P_{3/2}-(^3P)5d\ ^2P_{3/2}$

^aFrom an unpublished Xenon line list by Boyce, kindly put at our disposal by Humphreys (Ref. 11).

^bFrom the level values given in Table II by means of the Ritz combination principle. Only that part which differs from the observed is given.

TABLE II. Energy levels of Xe IV.

Designation	Energy (cm ⁻¹)	Percentage composition ^a
$5s^25p^3\ ^4S_{3/2}$	0.0	$86(5s^25p^3\ ^4S) + 11(5s^25p^3\ ^2P)$
$5s^25p^3\ ^2D_{3/2}$	13 268.0	$76(5s^25p^3\ ^2D) + 15(5s^25p^3\ ^2P) + 9(5s^25p^3\ ^4S)$
$5s^25p^3\ ^2D_{5/2}$	17 512.1	100
$5s^25p^3\ ^2P_{1/2}$	28 036.0	100
$5s^25p^3\ ^2P_{3/2}$	35 650.4	$74(5s^25p^3\ ^2P) + 21(5s^25p^3\ ^2D) + 5(5s^25p^3\ ^4S)$
$5s5p^4\ ^4P_{5/2}$	99 663.8	$85(5s5p^4\ ^4P) + 10[5s^25p^2(^3P)5d\ ^4P]$
$5s5p^4\ ^4P_{3/2}$	106 923.3	$85(5s5p^4\ ^4P) + 11[5s^25p^2(^3P)5d\ ^4P]$
$5s5p^4\ ^4P_{1/2}$	109 254.4	$83(5s5p^4\ ^4P) + 11[5s^25p^2(^3P)5d\ ^4P] + 5(5s5p^4\ ^2S)$
$5s5p^4\ ^2D_{3/2}$	121 928.8	$61(5s5p^4\ ^2D) + 18[5s^25p^2(^1D)5d\ ^2D] + 6[5s^25p^2(^3P)5d\ ^2P]$
$5s5p^4\ ^2D_{5/2}$	125 474.9	$70(5s5p^4\ ^2D) + 21[5s^25p^2(^1D)5d\ ^2D]$
$5s^25p^2(^3P)5d\ ^2P_{3/2}$	133 027.1	$33[5s^25p^2(^3P)5d\ ^2P] + 21[5s^25p^2(^3P)5d\ ^4F]$ $+ 12(5s5p^4\ ^2P) + 12(5s5p^4\ ^2D) + 11[5s^25p^2(^3P)5d\ ^4D]$
$5s^25p^2(^3P)5d\ ^4F_{3/2}$	134 980.6	$62[5s^25p^2(^3P)5d\ ^4F] + 20[5s^25p^2(^3P)5d\ ^2P] + 12(5s5p^4\ ^2P)$
$5s^25p^2(^3P)5d\ ^4F_{5/2}$	136 495.7	$71[5s^25p^2(^3P)5d\ ^4F] + 20[5s^25p^2(^3P)5d\ ^4D]$
$5s5p^4\ ^2P_{1/2}$	136 795.8	$22(5s5p^4\ ^2P) + 36[5s^25p^2(^3P)5d\ ^2P]$ $+ 23(5s5p^4\ ^2S) + 8[5s^25p^2(^3P)5d\ ^4D] + 8[5s^25p^2(^1D)5d\ ^2S]$

TABLE II. (Continued).

Designation	Energy (cm^{-1})	Percentage composition ^a
$5s^25p^2(^3P)5d^4F_{7/2}$	141 625.1 ^b	$82[5s^25p^2(^3P)5d^4F] + 16[5s^25p^2(^3P)5d^4D]$
$5s^25p^2(^1D)5d^2F_{5/2}$	141 824.4 ^b	$37[5s^25p^2(^1D)5d^2F] + 30[5s^25p^2(^3P)5d^2F]$ $+ 16[5s^25p^2(^3P)5d^4F] + 15[5s^25p^2(^3P)5d^4D]$
$5s^25p^2(^3P)5d^4D_{7/2}$	145 011.3 ^b	$41[5s^25p^2(^3P)5d^4D] + 30[5s^25p^2(^1D)5d^2F]$ $+ 16[5s^25p^2(^3P)5d^2F] + 8[5s^25p^2(^3P)5d^4F]$
$5s^25p^2(^3P)5d^4D_{1/2}$	145 105.7	$62[5s^25p^2(^3P)5d^4D] + 24(5s5p^4^2S) + 8[5s^25p^2(^1D)5d^2S]$
$5s^25p^2(^3P)5d^4F_{9/2}$	145 991.6 ^b	$86[5s^25p^2(^3P)5d^4F] + 14[5s^25p^2(^1D)5d^2G]$
$5s^25p^2(^3P)5d^4D_{3/2}$	146 206.4	$83[5s^25p^2(^3P)5d^4D] + 8[5s^25p^2(^3P)5d^4F]$
$5s^25p^2(^3P)5d^4D_{5/2}$	148 685.2	$55[5s^25p^2(^3P)5d^4D] + 16[5s^25p^2(^3P)5d^2F]$ $+ 14[5s^25p^2(^1D)5d^2F] + 10[5s^25p^2(^3P)5d^4F]$
$5s5p^4^2S_{1/2}$	150 737.4	$24(5s5p^4^2S) + 28[5s^25p^2(^3P)5d^4D]$ $+ 27[5s^25p^2(^3P)5d^2P] + 11(5s5p^4^2P) + 7[5s^25p^2(^1D)5d^2S]$
$5s^25p^2(^3P)6s^4P_{1/2}$	154 532.0	$75[5s^25p^2(^3P)6s^4P] + 13[5s^25p^2(^3P)6s^2P] + 9[5s^25p^2(^1S)6s^2S]$
$5s^25p^2(^3P)5d^2F_{7/2}$	155 863.9 ^b	$22[5s^25p^2(^3P)5d^2F] + 39[5s^25p^2(^3P)5d^4D] + 16[5s^25p^2(^1D)5d^2G]$ $+ 14[5s^25p^2(^1D)5d^2F] + 9[5s^25p^2(^3P)5d^4F]$
$5s^25p^2(^3P)5d^4P_{5/2}$	159 643.1	$78[5s^25p^2(^3P)5d^4P] + 5[5s^25p^2(^3P)5d^4D]$
$5s^25p^2(^3P)5d^4P_{3/2}$	161 434.1	$40[5s^25p^2(^3P)5d^4P] + 18[5s^25p^2(^3P)5d^2D] + 15[5s^25p^2(^1D)5d^2P]$ $+ 11[5s^25p^2(^1S)5d^2D] + 5(5s5p^4^4P)$
$5s^25p^2(^3P)5d^2D_{3/2}$	163 596.2	$33[5s^25p^2(^3P)5d^2D] + 23[5s^25p^2(^3P)5d^4P]$ $+ 17[5s^25p^2(^1S)5d^2D] + 10(5s5p^4^2P)$
$5s^25p^2(^3P)6s^4P_{3/2}$	165 280.5	$82[5s^25p^2(^3P)6s^4P] + 7[5s^25p^2(^1D)5d^2P] + 7[5s^25p^2(^3P)6s^2P]$
$5s^25p^2(^3P)6s^2P_{1/2}$	167 206.9	$58[5s^25p^2(^3P)6s^2P] + 18[5s^25p^2(^3P)6s^4P]$ $+ 11[5s^25p^2(^3P)5d^4P] + 7[5s^25p^2(^1D)5d^2P]$
$5s^25p^2(^3P)5d^2D_{5/2}$	169 001.8 ^b	$49[5s^25p^2(^3P)5d^2D] + 20[5s^25p^2(^3P)6s^4P]$ $+ 11[5s^25p^2(^1D)6s^2D] + 8[5s^25p^2(^3P)5d^2F]$
$5s^25p^2(^3P)6s^4P_{5/2}$	170 132.6	$49[5s^25p^2(^3P)6s^4P] + 17[5s^25p^2(^3P)5d^2D]$ $+ 15[5s^25p^2(^1D)6s^2D] + 7[5s^25p^2(^1D)5d^2D]$
$5s^25p^2(^1D)5d^2P_{3/2}$	170 490.0	$23[5s^25p^2(^1D)5d^2P] + 35(5s5p^4^2P) + 12[5s^25p^2(^3P)5d^4P]$ $+ 9[5s^25p^2(^1D)5d^2D] + 9[5s^25p^2(^3P)5d^2P]$
$5s^25p^2(^1D)5d^2P_{1/2}$	172 892.4 ^b	$59[5s^25p^2(^1D)5d^2P] + 14(5s5p^4^2P)$ $+ 12[5s^25p^2(^3P)5d^4P] + 10[5s^25p^2(^3P)6s^2P]$
$5s^25p^2(^3P)6s^2P_{3/2}$	173 222.0	$58[5s^25p^2(^3P)6s^2P] + 29[5s^25p^2(^1D)6s^2D]$
$5s^25p^2(^1D)5d^2D_{5/2}$	179 002.1	$50[5s^25p^2(^1D)5d^2D] + 12(5s5p^4^2D) + 9[5s^25p^2(^3P)5d^2F]$ $+ 8[5s^25p^2(^1D)5d^2F] + 7[5s^25p^2(^3P)6s^4P]$
$5s^25p^2(^1D)5d^2D_{3/2}$	186 050.3	$20[5s^25p^2(^1D)5d^2D] + 23[5s^25p^2(^1D)6s^2D] + 16[5s^25p^2(^3P)5d^2P]$ $+ 16[5s^25p^2(^1D)5d^2P] + 13(5s^25p^4^2P) + 7(5s5p^4^2D)$

^aPercentages lower than 5% are omitted. The average LS purity of the $5s5p^4$, $5s^25p^2(5d+6s)$ is 58%.

^bNew level.

$5s^25p^26p$ configuration, except for the levels at 154 532, 170 132, 179 001, and 186 052 cm^{-1} , which were previously observed by Boyce and Humphreys,¹ where we mainly observed transitions with the ground-state configuration. The levels corresponding to the $5s^25p^26p$ configuration will be discussed elsewhere.

The energy-level values shown in Table II were determined in an iterative procedure that takes into account the wave numbers of the observed lines, weighted according to their estimated uncertainties. All level designations are in LS notation, and in the same table we present

the percentage composition of the levels in LS coupling.

We confirm the energy levels of the $5s5p^4$ configuration previously classified by Di Rocco *et al.*,² except for the level at 134 980.1 cm^{-1} , which is now designated as $5s^25p^25d(^3P)^4F_{3/2}$ in accordance with the percentage composition of the level for LS coupling.

All levels presented in Table II are now classified through a least-squares fit of the observed levels. So we have classified 23 energy levels belonging to the $5s^25p^25d$ and $5s^25p^26s$ configurations.

THEORETICAL INTERPRETATION

Theoretical calculations were made at the Department of Physics, University of Lund, using a vax computer, model Vax/VMS version V5.2 from Digital Equipment Corporation.

Theoretical predictions of the energy levels of the configurations have been used in the analysis of the spectra. The predictions were obtained by diagonalizing the energy matrices with appropriate Hartree-Fock⁸ (HF) values for the energy parameters. For this purpose the computer code developed by Cowan⁹ was used.

In the initial phase of the analysis we did not take into account the interactions between the $5s5p^4$, $5s^25p^25s$, and $5s^25p^26s$ configurations. The results showed the necessity of considering configuration-interaction integrals. The $5s5p^4$ - $5s^25p^26s$ configuration interaction can be neglected because its HF value is 543.0 cm^{-1} , but the $5s5p^4$ - $5s^25p^25d$ interaction is very strong since its Hartree-Fock value for the interaction integral is $53\,723.5$

cm^{-1} . In spite of considering the interactions, the interpretation of the configuration-level structures using a least-squares fit was not good.

In order to obtain a better interpretation of the levels it was necessary to introduce the $5s^25p^26d$ configuration that forms a Rydberg series with the $5s^25p^25d$ configuration. The $5s5p^4$ - $5s^25p^26d$ configuration interaction has a value of $21\,420.0\text{ cm}^{-1}$. On the other side, the $5s^25p^25d$ - $5s^25p^26d$ Rydberg-series configuration interaction has, for one of the integrals, the Hartree-Fock value $16\,500.0\text{ cm}^{-1}$. Calculations considering the introduction of Rydberg-series configuration interactions in Xe III were made by Persson *et al.*¹⁰ The results of the parametric calculations are present in Table III. In our case, all the experimental level values of the $5s^25p^26d$ configuration are unknown, and due to this, all parameters of this configuration were held fixed in the least-squares-fit calculations. All the configuration-interaction integrals were held fixed in the calculation at scaled Hartree-Fock values. The scaled Hartree-Fock factor is

TABLE III. Energy parameters (cm^{-1}) for the $5s5p^4$, $5s^25p^2(5d+6s+6d)$ configurations of Xe IV. V represents the value in column four divided by the value in column three.

Configuration	Parameter	HF value	Fitted value ^a	V
$5s5p^4$	E_{av}	116 163	$137\,902\pm 274$	1.187 ± 0.002
	$F^2(5p, 5p)$	53 058	$44\,580\pm 2019$	0.840 ± 0.038
	ζ_{5p}	9 470	$8\,836\pm 465$	0.933 ± 0.049
	$G^1(5s, 5p)$	69 722	$56\,145\pm 979$	0.805 ± 0.014
$5s^25p^25d$	E_{av}	141 182	$158\,033\pm 136$	1.119 ± 0.001
	$F^2(5p, 5p)$	53 339	$34\,832\pm 1473$	0.653 ± 0.028
	ζ_{5p}	9 639	$8\,857\pm 249$	0.919 ± 0.026
	ζ_{5d}	684	762 ± 164	1.114 ± 0.240
	$F^2(5p, 5d)$	39 919	$36\,251\pm 1039$	0.908 ± 0.026
	$G^1(5p, 5d)$	45 262	$31\,365\pm 414$	0.693 ± 0.009
	$G^3(5p, 5d)$	28 429	$25\,941\pm 1196$	0.912 ± 0.042
$5s^25p^26s$	E_{av}	158 554	$175\,432\pm 335$	1.106 ± 0.002
	$F^2(5p, 5p)$	53 878	$44\,941\pm 3839$	0.834 ± 0.071
	ζ_{5p}	9 925	$9\,935\pm 269$	1.001 ± 0.027
	$G^1(5p, 6s)$	6 361	$5\,777\pm 602$	0.908 ± 0.095
$5s^25p^26d$	E_{av}	235 367	276 902 (fix)	1.176
	$F^2(5p, 5p)$	54 529	46 350 (fix)	0.850
	ζ_{5p}	10 137	9 630 (fix)	0.950
	ζ_{6d}	201	191 (fix)	0.950
	$F^2(5p, 6d)$	11 566	9 831 (fix)	0.850
	$G^1(5p, 6d)$	7 111	6 044 (fix)	0.850
	$G^3(5p, 6d)$	5 058	4 299 (fix)	0.850
CI integrals				
$5s5p^4$ - $5s^25p^25d$	$R^1(5p5p, 5s5d)$	53 724	43341 (fix)	0.807
$5s5p^4$ - $5s^25p^26s$	$R^1(5p5p, 5s6s)$	543	462 (fix)	0.850
$5s5p^4$ - $5s^25p^26d$	$R^1(5p5p, 5s6d)$	21 420	18207 (fix)	0.850
$5s^25p^25d$ - $5s^25p^26s$	$R^2(5p5d, 5p6s)$	-12 211	-10 379 (fix)	0.850
$5s^25p^25d$ - $5s^25p^26s$	$R^1(5p5d, 5p6s)$	-4 221	-3 588 (fix)	0.850
$5s^25p^25d$ - $5s^25p^26d$	$R^0(5p5d, 5p6d)$	0	0 (fix)	
$5s^25p^25d$ - $5s^25p^26d$	$R^2(5p5d, 5p6d)$	11 451	9 733 (fix)	0.850
$5s^25p^25d$ - $5s^25p^26d$	$R^1(5p5d, 5p6d)$	16 500	14 025 (fix)	0.850
$5s^25p^25d$ - $5s^25p^26d$	$R^3(5p5d, 5p6d)$	10 846	9 219 (fix)	0.850
$5s^25p^26s$ - $5s^25p^26d$	$R^2(5p6s, 5p6d)$	5 688	4 835 (fix)	0.850
$5s^25p^26s$ - $5s^25p^26d$	$R^1(5p6s, 5p6d)$	780	663 (fix)	0.850

^aThe rms deviation of the fit is 325 cm^{-1} for 31 observed levels.

0.85 in all the integrals, except for $5s5p^4-5s^25p^25d$ where the value is 0.81. For the configurations $5s5p^4$ and $5s^25p^26s$ all parameters were let free. The standard deviation for the 31 observed levels is 325 cm^{-1} .

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