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Extended analysis of the six-times ionized xenon, Xe VII

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Abstract. The spectrum of six-times ionized xenon, Xe VII, has been studied in the 270−6 500 Å using a pulsed discharge. 110 new classified lines are reported. Ten levels belonging to the odd parity configurations and four belonging to the even configurations have been determined. To obtain the energy parameters Hartree-Fock relativistic calculations were used. Least-squares parametric calculation has been carried out to study the fit between experimental and theoretical values.

PACS. 32.30.Jc Visible and ultraviolet spectra – 52.80.Yr Discharges for spectral sources (including inductively coupled plasma)

1 Introduction

Cadmium-like xenon, Xe VII, has the ground configuration $5s^2$. Previous works were carried out by different groups of researcher [1–6] who used various experimental methods such as beam-foil spectroscopy, spark-light sources, laser-produced plasma, theta-pinches, etc. A study of the $5p5d$ configuration by Cavalcanti *et al.* was in the last time reported [7]. Larsson *et al.* [8] obtained energy levels of the $5s6s$, $5s5d$ and $5p^2$, and $5s4f$ configurations by collision-based spectroscopy. Using the same kind of excitation, Wang *et al.* [9] extended the Larsson's work to include the $5s(6p+7p)$ and $5s(6d+7s)$ configurations. New results for ions in the Cd-like isoelectronic sequence [10–14] were recently published.

In this work we report additional experimental results for the Xe VII spectrum in the VUV region. In these results we include 14 new energy levels and 110 new transitions. The accuracy of the confirmed values of the known energy levels reported in references [8,9] were also improved. This study is a continuation of our investigations of different xenon ion spectra using gases pulsed electrical discharges ([15–19], and references therein). Hartree-Fock calculations including relativistic corrections and interpolation through the Cd I isoelectronic sequence were used to predict energy level values and transitions. It is expected that the spectroscopy of highly ionized xenon will be of interest for future diagnostics in the International Tokamak for Experimental Research, ITER ([7], and references therein).

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2 Experiment

A light source specially built at CIOp to study highly ionized noble gases, based on the discharge tube reported by Gallardo *et al.* [19], was used in this work. It is a 110 cm long Pyrex tube with an inner diameter of 3 mm. A bank of low-inductance capacitors varying between 40 and 240 nF charged up to 20 kV through the tube, was used to produce the gas excitation. Below 2 000 Å the light radiation was analysed using a 3 m normal incidence vacuum spectrograph with a plate factor in the first diffraction order of 2.77 Å mm^{-1}. Kodak SWR plates were used to record the spectra and C, N, O and known lines of Xe provided internal wavelength standards. To record the spectra in the UV–visible region, a 3.4 m Ebert plane grating spectrograph at CIOp 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 and third diffraction order. Thorium lines from an electrodeless discharge were superimposed on the spectrograms and served as reference lines [20,21].

To measure the spectrograms a photoelectric semiautomatic Grant comparator was used. We studied the behaviour of the spectral line intensities as a function of pressure and discharge voltage to distinguish between different states of ionisation. In our spectrograms of xenon, as the pressure decreases, higher ionic species tend to appear [16]. In this way, observing the behaviour of the spectral lines and using known lines of Xe VII, we were able to distinguish the different ionic states of our xenon spectra. The accuracy of the wavelength values is estimated to be ±0.02 Å in the VUV region. In the UV–visible range the uncertainty is estimated to be ±0.01 Å in the first diffraction order.

Table 1. New and adjusted energy values of the $5s^2$, $5p^2$, $5s5d$, $5s6d$, $5s6s$, $5s7s$ and $5s6p$, $5s7p$, $5p5d$, $5s5f$ configurations of Xe VII.

Designation		$E_{\exp}(\mathrm{cm}^{-1})^{a}$	$E_{\mathrm{calc}}(\mathrm{cm}^{-1})^{b}$	Percentage composition[c]
$5s^2$	$^1S_0$	0	0	98
$5p^2$	$^1S_0$	278 113[n]	278 073	90 $5p^2$ ^{3}P + 9 $5p^2$ ^{1}S
	$^1D_2$	236 100	236 267	55 $5p^2$ ^{1}D + 38 $5p^2$ ^{3}P + 6 $5s5d$ ^{1}D
$5s5d$	$^1D_2$	307 545	307 532	83 $5s5d$ ^{1}D + 10 $5p^2$ ^{1}D
$5s6d$	$^3D_1$	475 967	475 933	100
	$^3D_2$	476 239	476 229	99
	$^3D_3$	476 784	476 827	100
	$^1D_2$	479 665[n]	479 665	96
$5s6s$	$^1S_0$	363 511[n]	363 511	100
	$^3S_1$	354 833	354833	100
$5s7s$	$^1S_0$	510 731[n]	510 736	100
	$^3S_1$	506 240	506 230	100
$5s6p$	$^3P_0$	400 486	400 448	98
	$^3P_1$	400 876	400 912	77 $5s6p$ ^{3}P + 21 $5s6p$ ^{1}P
	$^3P_2$	408 088	407 973	69 $5s6p$ ^{3}P + 18 $5p5d$ ^{1}D + 6 $5p5d$ ^{3}D
	$^1P_1$	407 801	407 878	70 $5s6p$ ^{1}P + 14 $5s6p$ ^{3}P + 8 $5p5d$ ^{3}D +5 $5p5d$ ^{3}D
$5p5d$	$^3F_2$	394 360[n]	394 488	80 $5p5d$ ^{3}F + 17 $5p5d$ ^{1}D
	$^3F_3$	402 505[n]	402 230	87 $5p5d$ ^{3}F + 8 $5p5d$ ^{3}D
	$^3F_4$	414 074[n]	414 005	98
	$^1F_3$	438 427	438 837	78 $5p5d$ ^{1}F + 13 $5s$ ^{1}F + 7 $5p5d$ ^{3}D
	$^3D_1$	410 500[n]	410 636	61 $5p5d$ ^{3}D + 15 $5p5d$ ^{3}P + 9 $5s6p$^{1}P + 8 $5p5d$ ^{1}P + $5s6p$ ^{3}P
	$^3D_2$	418 483[n]	418 287	37 $5p5d$ ^{1}D + 34 $5p5d$ ^{3}D + 17 $5p5d$ ^{3}P + 10 $5p5d$ ^{3}F
	$^3D_3$	423 840	423 829	84 $5p5d$ ^{3}D + 11 $5p5d$ ^{3}F
	$^1D_2$		404 209	29 $5p5d$ ^{3}P + 28 $5s6p$ ^{3}P + 24 $5p5d$ ^{1}D + 13 $5p5d$ ^{3}D + 6 $5p5d$ ^{3}F
	$^3P_0$	424 921[n]	424 982	98
	$^3P_1$	425 406	425 251	74 $5p5d$ ^{3}P + 24 $5p5d$ ^{3}D
	$^3P_2$	426 105[n]	425 898	50 $5p5d$ ^{3}P + 45 $5p5d$ ^{3}D
	$^1P_1$	443 192	442 955	89 $5p5d$ ^{1}P + 6 $5p5d$ ^{3}D
$5s5f$	$^3F_2$	463 954[n]	463 751	99
	$^3F_3$	463 810[n]	463 955	99
	$^3F_4$		464 227	98
	$^1F_3$		468 322	87
$5s7p$	$^3P_0$	527 044	526 884	100
	$^3P_1$	527 500	527 361	91 $5s7p$ ^{3}P + 9 $5s7p$ ^{1}P
	$^3P_2$	529 348	529 620	99
	$^1P_1$	531 766[n]	531 779	90 $5s7p$ ^{1}P + 8 $5s7p$ ^{3}P

[a] Uncertainties of the adjusted experimental energy level values less than 4 cm^{-1}.
[b] Calculated energy level values obtained using the fitted energy parameters.
[c] Percentages below 5% have been omitted.
[n] New energy values.

3 Analysis

Theoretical predictions of the structure of the configurations were used in the analysis. The predictions were obtained by diagonalizing the energy matrices with appropriately scaled relativistic Hartree-Fock (HFR) values for the energy parameters. The computer code developed by Cowan [22] was used. Comparisons along the Cd I isoelectronic sequence were also used.

Table 2 shows the new classified transitions. The intensities of the transitions are visually estimations of plate blackening.

The adjusted experimental energy level values derived from the observed lines are given in Table 1. The level values were determined in an iterative procedure where the wavenumbers of the observed lines are weighted in accordance to their estimated uncertainties. In our case the uncertainties of the adjusted experimental energy level values are generally less than 4 cm^{-1}. All level designations

Table 2. Classified lines of Xe VII.

Intensity	λ_{obs} (Å) in vacuum	σ_{obs} (cm^{-1})	σ_{cal} (cm^{-1})^b	Transition
1	360.35	277 508	495	$5p^2\ ^3P_2$–$5s7p\ ^3P_2$
2	409.83	244 004	3 994	$5s5d\ ^3D_1$–$5s7p\ ^1P_1$
1	411.42	243 061	53	$5s5d\ ^3D_2$–$5s7p\ ^1P_1$
1	413.95	241 576	5	$5s5d\ ^3D_1$–$5s7p\ ^3P_2$
1	436.18	229 263	72	$5p^2\ ^3P_1$–$5s5f\ ^3F_2$
1	446.01	224 210	21	$5s5d\ ^1D_2$–$5s7p\ ^1P_1$
1	450.85	221 803	3	$5s5d\ ^1D_2$–$5s7p\ ^3P_2$
1	454.03	220 250	0	$5s5p\ ^1P_1$–$5s6s\ ^1S_0$
10	482.88	207 091	2	$5p^2\ ^1D_2$–$5p5d\ ^1P_1$
10	482.88	207 091	4	$5s5p\ ^3P_1$–$5s5d\ ^1D_2$
8	494.25	202 327	7	$5p^2\ ^1D_2$–$5p5d\ ^1F_3$
1	522.66	191 329	39	$5p^2\ ^3P_2$–$5p5d\ ^1P_1$
4	524.30	190 731	24	$5p^2\ ^3P_1$–$5p5d\ ^3P_1$
4	526.33	190 005	89 995	$5p^2\ ^1D_2$–$5p5d\ ^3P_2$
4	528.24	189 308	6	$5p^2\ ^1D_2$–$5p5d\ ^3P_1$
7	543.10	184 128	7	$5p^2\ ^3P_0$–$5s6p\ ^1P_1$
1	544.08	183 797	801	$5p^2\ ^3P_1$–$5p5d\ ^3D_2$
2	567.59	176 184	2	$5s5d\ ^3D_1$–$5s5f\ ^3F_2$
4	570.63	175 245	1	$5s5d\ ^3D_2$–$5s5f\ ^3F_2$
3	571.10	175 101	097	$5s5d\ ^3D_2$–$5s5f\ ^3F_3$
1	573.38	174 404	0	$5p^2\ ^1D_2$–$5p5d\ ^3D_1$
1	573.86	174 259	2	$5p^2\ ^3P_2$–$5p5d\ ^3P_2$
5	574.38	174 101	098	$5s5p\ ^3P_2$–$5s5d\ ^3D_1$
4	576.48	173 467	71	$5s5d\ ^3D_3$–$5s5f\ ^3F_3$
8	577.63	173 121	19	$5p^2\ ^3P_1$–$5s6p\ ^1P_1$
3	579.15	172 667	7	$5s6s\ ^3S_1$–$5s7p\ ^3P_1$
4	580.66	172 218	1	$5s6s\ ^3S_1$–$5s7p\ ^3P_0$
7	694.00	160 406	5	$5p^2\ ^1D_2$–$5p5d\ ^3F_3$
2	601.71	166 193	4	$5p^2\ ^3P_1$–$5s6p\ ^3P_1$
3	605.79	165 074	9	$5p^2\ ^1S_0$–$5p5d\ ^1P_1$
2	639.37	156 403	9	$5s5d\ ^1D_2$–$5s5f\ ^3F_2$
4	639.94	156 265	5	$5s5d\ ^1D_2$–$5s5f\ ^3F_3$
4	640.03	156 243	35	$5p^2\ ^3P_2$–$5s6p\ ^3P_2$
1	671.02	149 027	3	$5p^2\ ^3P_2$–$5s6p\ ^3P_1$
4	675.28	148 087	8	$5s5d\ ^3D_3$–$5p5d\ ^1F_3$
5	687.53	145 448	52	$5s5p\ ^1P_1$–$5s5d\ ^3D_2$
5	691.98	144 513	1	$5s5p\ ^1P_1$–$5s5d\ ^3D_1$
4	701.74	142 503	7	$5p^2\ ^3P_2$–$5p5d\ ^3F_2$
1	727.85	137 391	2	$5s5d\ ^3D_2$–$5p5d\ ^3P_2$
1	729.11	137 154	49	$5s5d\ ^3D_1$–$5p5d\ ^3P_0$
5	731.56	136 694	4	$5s5d\ ^3D_2$–$5p5d\ ^3P_1$
8	737.21	135 647	7	$5s5d\ ^1D_2$–$5p5d\ ^1P_1$
8	737.21	135 647	9	$5s5p\ ^3P_1$–$5p^2\ ^1D_2$
3	741.56	134 851	2	$5s5p\ ^1P_1$–$5p^2\ ^1S_0$
8	749.03	133 506	1	$5s5d\ ^3D_3$–$5p5d\ ^3D_3$
7	764.02	130 887	2	$5s5d\ ^1D_2$–$5p5d\ ^1F_3$
4	765.02	130 716	1	$5s5d\ ^3D_1$–$5p5d\ ^3D_2$
5	770.62	129766	70	$5s5d\ ^3D_2$–$5p5d\ ^3D_2$
5	771.07	129 690	88	$5p^2\ ^1S_0$–$5s6p\ ^1P_1$
7	780.34	128 149	4	$5s5d\ ^3D_3$–$5p5d\ ^3D_2$

Table 2. *Continued.*

Intensity	λ_{obs} (Å) in vacuum	σ_{obs} (cm^{-1})	σ_{cal} (cm^{-1})^{b}	Transition
3	808.18	123 735	5	$5s5d\ ^3D_3$–$5p5d\ ^3F_4$
3	814.81	122 728	8	$5s5d\ ^3D_1$–$5p5d\ ^3D_1$
4	831.16	120 314	6	$5s5d\ ^3D_1$–$5s6p\ ^3P_2$
5	837.20	119 375	6	$5s5d\ ^3D_2$–$5s6p\ ^3P_2$
4	839.75	119 083	8	$5s5d\ ^3D_2$–$5s6p\ ^1P_1$
2	848.43	117 865	1	$5s5d\ ^1D_2$–$5p5d\ ^3P_1$
6	849.26	117 750	49	$5s5d\ ^3D_3$–$5s6p\ ^3P_2$
4	874.69	114 326	34	$5s5d\ ^3D_2$–$5p5d\ ^1D_2$
6	884.13	113 106	4	$5s5d\ ^3D_1$–$5s6p\ ^3P_1$
6	887.20	112 714	4	$5s5d\ ^3D_1$–$5s6p\ ^3P_0$
5	891.55	112 164	6	$5s5d\ ^3D_3$–$5p5d\ ^3F_3$
5	891.55	112 164	4	$5s5d\ ^3D_2$–$5s6p\ ^3P_1$
3	938.23	106 584	8	$5s5d\ ^3D_1$–$5p5d\ ^3F_2$
2	946.49	105 654	47	$5s5d\ ^3D_2$–$5p5d\ ^3F_2$
2	971.52	102 932	0	$5s6p\ ^1P_1$–$5s7s\ ^1S_0$
3	1044.54	95 736	40	$5p5d\ ^3D_1$–$5s7s\ ^3S_1$
6	1213.29	82 421	4	$5p5d\ ^3F_2$–$5s6d\ ^3D_3$
4	1225.46	81 602	7	$5p5d\ ^3F_2$–$5s6d\ ^3D_1$
4	1 229.83	81 312	9	$5p5d\ ^3P_0$–$5s7s\ ^3S_1$
7	1 243.58	80 413	3	$5s5p\ ^1P_1$–$5p^2\ ^3P_0$
2	1 247.90	80 135	5	$5p5d\ ^3P_2$–$5s7s\ ^3S_1$
2	1 254.92	79 686	1	$5s6s\ ^1S_0$–$5p5d\ ^1P_1$
3	1 296.05	77 158	60	$5p5d\ ^3F_3$–$5s6d\ ^1D_2$
2	1 326.93	75 362	3	$5s6p\ ^3P_1$–$5s6d\ ^3D_2$
6	1 331.63	75 096	1	$5s6p\ ^3P_1$–$5s6d\ ^3D_1$
2	1 356.15	73 738	4	$5p5d\ ^3F_3$–$5s6d\ ^3D_2$
4	1 391.49	71 865	4	$5s6p\ ^1P_1$–$5s6d\ ^1D_2$
2	1 396.96	71 584	77	$5s6p\ ^3P_2$–$5s6d\ ^1D_2$
4	1 426.72	70 091	88	$5s6s\ ^3S_1$–$5p5d\ ^3P_0$
2	1 445.81	69 165	5	$5p5d\ ^3D_1$–$5s6d\ ^1D_2$
3	1 455.68	68 696	6	$5s6p\ ^3P_2$–$5s6d\ ^3D_3$
2	1 460.95	68 449	38	$5s6p\ ^1P_1$–$5s6d\ ^3D_2$
4	1 473.25	67 877	9	$5s6p\ ^3P_2$–$5s6d\ ^3D_1$
2	1 480.57	67 542	39	$5p5d\ ^1P_1$–$5s7s\ ^1S_0$
8	1 527.40	65 471	67	$5p5d\ ^3D_1$–$5s6s\ ^3D_1$
6	1 586.00	63 052	48	$5p5d\ ^1P_1$–$5s7s\ ^3S_1$
10	1 594.63	62 711	0	$5p5d\ ^3F_4$–$5s6d\ ^3D_3$
2	1 615.65	61 895	5	$5s6s\ ^1S_0$–$5p5d\ ^3P_1$
8	1 715.23	58 301	1	$5p5d\ ^3D_2$–$5s6d\ ^3D_3$
8	1 731.39	57 757	8	$5p5d\ ^3D_2$–$5s6d\ ^3D_2$
7	1 791.17	55 829	5	$5p5d\ ^3D_3$–$5s6d\ ^1D_2$
8	1 843.20	54 254	9	$5p5d\ ^3P_1$–$5s6d\ ^1D_2$
7	1 867.08	53 560	0	$5p5d\ ^3P_2$–$5s6d\ ^1D_2$
7	1 888.81	52 943	4	$5p5d\ ^3D_3$–$5s6d\ ^3D_3$
4	1 902.47	52 563	4	$5s6d\ ^3D_3$–$5s7p\ ^3P_2$
6	1 919.19	52 105	1	$5s6d\ ^1D_2$–$5s7p\ ^1P_1$
7	1 950.78	51 262	1	$5s6d\ ^3D_2$–$5s7p\ ^3P_1$
7	1 957.79	51 078	7	$5s6d\ ^3D_1$–$5s7p\ ^3P_0$
7	1 958.87	51 050	46	$5p5d\ ^3P_0$–$5s6d\ ^3D_1$
7	1 967.07	50 837	3	$5p5d\ ^3P_1$–$5s6d\ ^3D_2$

Table 2. *Continued.*

Intensity	$\lambda_{\rm obs}$ (Å) in vacuum	$\sigma_{\rm obs}$ (cm^{-1})	$\sigma_{\rm cal}$ (cm^{-1})$^{\rm b}$	Transition
5	1 973.41	50 674	9	$5p5d$ ^{3}P$_2$–$5s6d$ ^{3}D$_3$
3	1 994.59	50 136	9	$5p5d$ ^{3}P$_2$–$5s6d$ ^{3}D$_2$
8	2 090.27	47 841	35	$5s6d$ ^{1}D$_2$–$5s7p$ ^{3}P$_1$
2	2 128.01	46 992	89	$5s6s$ ^{1}S$_0$–$5p5d$ ^{3}D$_1$
	$\lambda_{\rm air}$			
5	2 257.13	44 290.5	0.0	$5s6s$ ^{1}S$_0$–$5s6p$ ^{1}P$_1$
9	3 916.42	25 526.3	6.0	$5s7s$ ^{3}S$_1$–$5s7p$ ^{1}P$_1$
4	4 326.35	23 107.7	8.0	$5s7s$ ^{3}S$_1$–$5s7p$ ^{3}P$_2$
2	4 702.32	21 260.2	0.0	$5s7s$ ^{3}S$_1$–$5s7p$ ^{3}P$_1$
8	4 752.68	21 034.9	5.0	$5s7s$ ^{1}S$_0$–$5s7p$ ^{1}P$_1$
12	4 805.44	20 804.0	4.0	$5s7p$ ^{3}P$_0$–$5s7s$ ^{3}S$_1$

Intensity, observed lines intensities from visual estimation.
[b] Calculated wavenumber. Only the last digits which differ from the observed ones are given.

in Table 1 are in LS notation, and in the same table we present the percentage composition of the levels.

In the even parity configurations the $5p^2$ ^{1}S$_0$ energy level value reported by Larsson *et al.* [8] was rejected, and we propose a new energy level in 278 113 cm^{-1}, supported by three new transitions with the $5s5p$ ^{1}P$_1$, $5s6p$ ^{1}P$_1$, and the $5p5d$ ^{1}P$_1$ energy levels respectively. The new $5s5d$ ^{1}D$_2$ energy level value proposed by Larsson *et al.* [8] was confirmed and adjusted by adding seven new transitions shown in Table 1. We reject the $5s6s$ ^{1}S$_0$ energy level value reported by these same authors and propose a new value in 363 511 cm^{-1}, supported by five new transitions with the $5s5p$ ^{1}P$_1$, $5s6p$ ^{1}P$_1$ and the $5p5d$ ^{1}P$_1$, ^{3}P$_1$ and ^{3}D$_1$ energy levels respectively. We establish a new $5s6d$ ^{1}D$_2$ energy level value in 479 665 cm^{-1}, supported by nine new transitions. We also establish a new $5s7s$ ^{1}S$_0$ energy level value in 510 731 cm^{-1}, supported by three new transitions.

In the odd parity configurations, all the previously known energy level values for the $5s5p$, $5s6p$, and $5s7p$ configurations were confirmed, and we propose a new $5s7p$ ^{1}P$_1$ energy level value in 531 766 cm^{-1} supported by six new transitions with the $5s5d$ ^{3}D$_1$, ^{3}D$_2$, $5s5d$ ^{1}D$_2$, $5s6d$ ^{1}D$_2$, and $5s7s$ ^{1}S$_0$, ^{3}S$_1$ energy levels. We establish two new $5s5f$ ^{3}F$_2$ and $5s5f$ ^{3}F$_3$ energy level values in 463 954 cm^{-1} and 463 810 cm^{-1} respectively, supported by the transitions shown in Table 1. We were not able to find transitions that permit to establish the $5s5f$ ^{3}F$_4$ and $5s5f$ ^{1}F$_3$ energy level values. We rejected the $5p5d$ ^{3}P$_2$ energy level value reported in the paper of reference [7], and propose a new value in 426 105 cm^{-1}, supported by seven transitions shown in Table 1. We also establish a new $5p5d$ ^{3}P$_0$ energy level value in 424 921 cm^{-1}, supported by four transitions shown in Table 1. The energy level values for the $5p5d$ ^{1}P$_1$, ^{1}F$_3$, ^{3}P$_1$, and ^{3}D$_3$ reported in the paper of reference [7] were confirmed.

We reject the $5p5d$ ^{3}D$_1$ and ^{3}D$_2$ energy level values reported in the work of reference [7], and propose new values in 410 500 cm^{-1} and 418 483 cm^{-1} respectively. These values are supported by six new transitions each other shown in Table 1. We also reject the energy level values reported in reference [7] for all the J values belonging to the $5p5d$ ^{3}F multiplet, and propose a new value in 394 360 cm^{-1} for the ^{3}F$_2$, a new value in 402 505 cm^{-1} for the ^{3}F$_3$, supported by five new transitions each other; and a new value in 414 074 cm^{-1} for the ^{3}F$_4$, supported by two transitions with the $5s5d$ ^{3}D$_3$ and the $5s6d$ ^{3}D$_3$ energy levels.

4 Discussion

When interpreting the observed energy-level structures we performed least-squares fits between the experimental energy-level values and the eigenvalues obtained when diagonalizing the energy matrices.

To study the even parity configuration theoretically we have considered preliminary the complete $5s^2 + 5p^2 + 5s(6s + 7s + 5d + 6d) + 5p(4f + 5f) + 5p6p + 4f^2 + 5d^2 + 4d^9 5s^2(6s + 5d)$ energy matrix, and we observed that the more high configurations and also the core excited ones interact with the configurations here analyzed. The results of the parametric calculations for the even configurations are presented in Table 3. We included in the fitting the $4f5p$ configuration in accordance with the procedure reported calculations along the isoelectronic sequence [13]. The scaled Hartree-Fock factor was 0.85 for all the parameters, except for ζ_{nl} and for E_{av} that was 0.95 and 1.00 respectively. In our case all of the experimental level values of the $4f5p$ configuration are unknown, and due to this, all parameters of this configuration were held fixed in the least-squares fit calculation. Besides, all the configuration interaction integrals were held fixed in the calculation, at 0.85 of their HF values, except for the $5s^2$–$5p^2$, $5p^2$–$5s5d$, $5p^2$–$5s6d$, $5s5d$–$5s6d$, and $5s6d$–$4f5p$, that were held fixed in the calculation at 0.70 of their HF values, in order to obtain a better parametric fit.

Ab initio calculations to study the odd parity configurations considering the $5s(5p + 6p + 7p) + 5s(4f + 5f) + 5p(5d + 6d) + 5p6s + 5d6p + 5d(4f + 5f) + 4d^9 5s^2 5p$ energy matrices were carried out. The results of the parametric

Table 3. Energy parameters (cm^{-1}) for the studied even parity configurations of XeVII.

Configuration	Parameter	HF value	Fitted value	F/HF(*)
$5s^2$	E_{av}	00	3667	
$5p^2$	E_{av}	238 723	246 066 ± 59	1.030 ± 0.001
	ζ_{5p}	10 573	1 1417 ± 64	1.079 ± 0.006
	$F^2(5p,5p)$	59 133	48 322 ± 318	0.817 ± 0.005
$5s5d$	E_{av}	283 684	293 692 ± 64	1.035 ± 0.001
	ζ_{5d}	849	1062 ± 65	1.250 ± 0.076
	$G^2(5s,5d)$	38 852	35 253 ± 402	0.907 ± 0.010
$5s6d$	E_{av}	467 624	476 872 ± 59	1.019 ± 0.001
	ζ_{6d}	381	362 (FIX)	0.950
	$G^2(5s,6d)$	9150	4915 ± 348	0.537 ± 0.038
$5s6s$	E_{av}	347 141	357020 ± 92	1.028 ± 0.001
	$G^0(5s,6s)$	5220	4353 ± 82	0.833 ± 0.015
$5s7s$	E_{av}	494 171	507326 ± 92	1.026 ± 0.001
	$G^0(5s,7s)$	1792	2193 ± 82	1.223 ± 0.045
$4f5p$	E_{av}	388 137	388 137 (FIX)	1.000
	ζ_{4f}	254	242 (FIX)	0.950
	ζ_{5p}	10 165	9657 (FIX)	0.950
	$F^2(4f,5p)$	51 236	43 551 (FIX)	0.850
	$G^2(4f,5p)$	35 088	29 825 (FIX)	0.850
	$G^4(4f,5p)$	26 040	22 134 (FIX)	0.850
Configuration interaction integrals				
$5s^2$–$5p^2$	$R^1(5s5s,5p5p)$	76 811	53 767 (FIX)	0.700
$5s^2$–$5s6s$	$R^0(5s5s,5s6s)$	3890	3307 (FIX)	0.850
$5s^2$–$5s7s$	$R^0(5s5s,5s7s)$	1899	1614 (FIX)	0.850
$5p^2$–$5s5d$	$R^1(5p5p,5s5d)$	64 976	45 483 (FIX)	0.700
$5p^2$–$5s6d$	$R^1(5p5p,5s6d)$	25 549	17 884 (FIX)	0.700
$5p^2$–$5s6s$	$R^1(5p5p,5s6s)$	−318	−271 (FIX)	0.850
$5p^2$–$5s7s$	$R^1(5p5p,5s7s)$	−1862	−1583 (FIX)	0.850
$5p^2$–$4f5p$	$R^2(5p5p,4f5p)$	−42 609	−36 218 (FIX)	0.850
$5s5d$–$5s6d$	$R^0(5s5d,5s6d)$	0	0 (FIX)	
	$R^2(5s5d,6d5s)$	17 211	12 048 (FIX)	0.700
$5s5d$–$4f5p$	$R^3(5s5d,4f5p)$	−30 636	−26 041 (FIX)	0.850
	$R^1(5s5d,5p4f)$	−37 604	−31 964 (FIX)	0.850
$5s6d$–$4f5p$	$R^3(5s6d,4f5p)$	−13 701	−9590 (FIX)	0.700
	$R^1(5s6d,5p4f)$	−14 362	−10 053 (FIX)	0.700
$5s7s$–$4f5p$	$R^0(5s7s,4f5p)$	0	0 (FIX)	
	$R^0(5s7s,5p4f)$	2990	2542 (FIX)	0.850

(*) Fitted value/Hartree-Fock value.
The standard deviation of the fit is 117 cm^{-1}.

calculations are showed in Table 4, where the $5s7p$ configuration and the rest of the fitted configurations reported in reference [13] are included. In our calculations the radial parameters belonging to the $4f5s$ and the $4d^95s^25p$ configuration were held fixed at 0.85, 0.95 and 1.00 for the G^k, ζ_{nl} and E_{av} respectively. In the $5s6p$ configuration the $G^1(5s,6p)$ integral was optimized and fixed at 0.25 of its HF value. This value is in good agreement with the extrapolated value obtained along the isoelectronic sequence, reported in reference [9]. All the configuration interaction integrals were fixed at 0.85 of their HF values, except for the $5s5p$–$5p5d$, and $5p5d-5s5f$ integrals, fixed at 0.70 and 0.75 respectively.

Table 4. Energy parameters (cm^{-1}) for the studied odd parity configurations of XeVII.

Configuration	Parameter	HF value	Fitted value	F/HF
$5s5p$	E_{av}	108 320	117 703 ± 153	1.086 ± 0.001
	ζ_{5p}	10 652	11 681 ± 244	1.096 ± 0.022
	$G^1(5s,5p)$	76 823	56 556 ± 573	0.736 ± 0.007
$5s6p$	E_{av}	396 096	405 481 ± 192	1.023 ± 0.001
	ζ_{6p}	3972	4296 ± 230	1.081 ± 0.058
	$G^1(5s,6p)$	8585	2146 (FIX)	0.250
$5s7p$	E_{av}	518 487	529 360 ± 141	1.021 ± 0.001
	ζ_{7p}	1987	1800 (FIX)	0.900
	$G^1(5s,7p)$	3177	4122 ± 551	1.297 ± 0.173
$5p5d$	E_{av}	406 352	417 867 ± 103	1.028 ± 0.001
	ζ_{5p}	10 759	12 377 ± 261	1.150 ± 0.024
	ζ_{5d}	866	970 ± 173	1.120 ± 0.199
	$F^2(5p,5d)$	49 801	32 505 ± 976	0.652 ± 0.019
	$G^1(5p,5d)$	58 636	37 310 ± 495	0.636 ± 0.008
	$G^3(5p,5d)$	37 484	22 037 ± 1132	0.587 ± 0.030
$4f5s$	E_{av}	268 590	268 590 (FIX)	1.000
	ζ_{4f}	248	235 (FIX)	0.950
	$G^3(4f,5s)$	36 157	30 733(FIX)	0.850
$5s5f$	E_{av}	452 417	463 602 ± 199	1.024 ± 0.001
	ζ_{5f}	89	85 (FIX)	0.950
	$G^3(5s,5f)$	4471	3800 (FIX)	0.850
$4d^95s^25p$	E_{av}	532 110	540 110 (FIX)	1.015
	ζ_{4d}	6274	5960 (FIX)	0.950
	ζ_{5p}	11 505	10 930 (FIX)	0.950
	$F^2(5p,5d)$	41 955	35 662 (FIX)	0.850
	$G^1(5p,5d)$	12 587	10 699 (FIX)	0.850
	$G^3(5p,5d)$	12 281	10 438 (FIX)	0.850
Configuration interaction integrals				
$5s5p$–$5s6p$	$R^0(5s5p,5s6p)$	3246	2759 (FIX)	0.850
	$R^1(5s5p,6p5s)$	19 080	16 218 (FIX)	0.850
$5s5p$–$5s7p$	$R^0(5s5p,5s7p)$	1644	1397 (FIX)	0.850
	$R^1(5s5p,7p5s)$	9589	8151 (FIX)	0.850
$5s5p$–$5p5d$	$R^1(5s5p,5p5d)$	65 650	45 955 (FIX)	0.700
	$R^2(5s5p,5d5p)$	48 308	41 062 (FIX)	0.850
$5s5p$–$4d^95s^25p$	$R^2(4d4d,4d5s)$	−8155	−6931(FIX)	0.850
	$R^2(4d5p,5s5p)$	−22 705	−19 299 (FIX)	0.850
	$R^1(4d5p,5p5s)$	−20 004	−17 004 (FIX)	0.850
$5s6p$–$5s7p$	$R^0(5s6p,5s6p)$	0	0 (FIX)	
	$R^1(5s6p,6p5s)$	5095	4331 (FIX)	0.850
$5s6p$–$5p5d$	$R^1(5s6p,5p5d)$	−3559	−3025 (FIX)	0.850
	$R^2(5s6p,5d5p)$	6469	5498 (FIX)	0.850
$5s6p$–$4d^95s^25p$	$R^2(4d6p,5s5p)$	−5936	−5046 (FIX)	0.850
	$R^1(4d6p,5s5p)$	−4762	−4047 (FIX)	0.850
$5s7p$–$5p5d$	$R^1(5s7p,5p5d)$	−3106	−2640 (FIX)	0.850
	$R^2(5s7p,5p5d)$	1896	1611 (FIX)	0.850
$5s7p$–$4d^95s^25p$	$R^2(4d7p,5s5p)$	−2913	−2476 (FIX)	0.850
	$R^1(4d7p,5p5s)$	−2221	−1888 (FIX)	0.850
$5p5d$–$4f5s$	$R^2(5p5d,4f5s)$	−35 170	−29 894 (FIX)	0.850
	$R^1(5p5d,5s4f)$	−39 041	−33 185 (FIX)	0.850
$5p5d$–$5s5f$	$R^1(5p5d,5s5f)$	29 021	21 766 (FIX)	0.750
	$R^2(5p5d,5f5s)$	10 765	9150 (FIX)	0.850
$5p5d$–$4d^95s^25p$	$R^2(4d5d,5s5s)$	−166 44	−14 148 (FIX)	0.850
$4f5s$–$5s5f$	$R^3(4f5s,5s5f)$	−125	−106 (FIX)	0.850
	$R^0(4f5s,5f5s)$	0	0 (FIX)	
$4f5s$–$4d^95s^25p$	$R^2(4d4f,5s5p)$	23 511	19 984 (FIX)	0.850
	$R^3(4d4f,5p5s)$	19 363	16 458 (FIX)	0.850
$5s5f$–$4d^95s^25p$	$R^2(4d5f,5s5p)$	454	386 (FIX)	0.850
	$R^3(4d5f,5p5s)$	2460	2091 (FIX)	0.850

The standard deviation of the fit is 279 cm^{-1}.

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