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Extended Analysis of Xe VII and Xe VIII¹

M. Raineri, M. Gallardo, J. Reyna Almandos, C. J. B. Pagan and R. Sarmiento

Abstract: A pulsed discharge light source to study the six and seven times ionized xenon spectra in the 419-4642 Å region was used. A set of 40 transitions of Xe VII and 25 transitions of Xe VIII were classified for the first time. We revised the values for the previously known energy levels and extended the analysis for Xe VII to 10 new energy levels belonging to 5s6d, 5s7s and 5s7p, 4d⁹5s²5p even and odd configurations, respectively. 7 new energy levels of the core excited configuration 4d⁹5s5d of Xe VIII are presented. For the prediction of the atomic parameters, energy levels and transition, relativistic Hartree–Fock calculations were used.

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Keywords: Atomic spectra, Energy levels, Capillary-pulsed discharge, Relativistic Hartree–Fock calculations

1. Introduction

The spectral analysis of several ions of xenon has implications for astronomy and laser studies. Various atomic parameters such as energy levels, oscillator strengths, transition probabilities and radiative lifetimes have many important astrophysical applications. Transition probabilities are needed for calculating the energy transport through the star in model atmospheres [1] and for direct analysis of stellar chemical compositions [2]. Xenon is a very rare element in the cosmos, observed in chemically peculiar stars [3] and in planetary nebulae [4]. Xe VI and Xe VII lines were observed in the ultraviolet spectrum of the hot DO-type white dwarf RE 0503-289 [5-6], in the first detection of xenon in this kind of star.

Xe VII belongs to the Cd isoelectronic sequence and has the ground configuration 5s². In the studies related with the stimulated emission of xenon, the understanding of the population mechanisms that affect the Xe VII laser action requires knowledge of the spectral analysis corresponding to this ion. Results for ions in the Cd-like isoelectronic sequence were published [7-17] and previous works about cadmium-like xenon were carried out by different groups of researchers [18-23], who used various experimental methods such as beam-foil spectroscopy, spark-light sources, laser-produced plasma, theta-pinches, etc. Larsson et al. [24] obtained energy levels of the 5s6s, 5s5d and 5p², and 5s4f configurations by collision-based spectroscopy. Using the

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same kind of excitation, Wang et al.[25] extended Larsson's work to include the $5s(6p + 7p)$ and $5s(6d + 7s)$ configurations. The study of the $5p5d$ configuration by Cavalcanti et al using a theta-pinch as light source [26], by Gallardo et al, reporting fourteen new energy levels and one hundred and ten new lines using a pulsed discharge [27], was made. After that, Churilov and Joshi [28] used two different light sources to study this ion and reported thirty nine new energy level values.

Seven times ionized xenon, Xe VIII, belongs to the Ag I isoelectronic sequence and its ground state is $5s^2S_{1/2}$. The spectrum of this ion has been investigated by many groups using different spectral sources, e.g., by beam foil spectroscopy [29], by use of an inductance-triggered spark as light source [30–32] by CBS [33,34] and by a discharge tube [35,36]. Thereby, the configurations $5s$ – $9s$, $5p$ – $9p$, $5d$ – $9d$, $4f$ – $9f$, $5g$ – $9g$, $6h$ – $9h$, $7i$ – $10i$, $8k$ – $10k$, $9l$ have been established. Also some levels of core excited $4d^95s5p$, $4d^95s6p$ and $4d^95s5f$ configurations have been determined. In addition to these analyses some authors [29,30,34] have also established quantum defects of Rydberg levels important to predict energies of unknown levels and to derive ionization energies and core polarizabilities. In the work of M. Gallardo et al [37], using a capillary light source, twenty-eight energy levels belonging to the series Rydberg configurations were adjusted and 38 new spectral lines were classified.

The experimental results on energy levels and transitions of Xe VII and Xe VIII spectrum were critically compiled by Saloman [38]. Lifetimes and transition probabilities on these ions were reported by Biemont et al [39].

In order to continue the study of the six and seven times ionized xenon spectrum, a new spectral analysis of these ions is presented in this work. This study is a continuation of our research on different xenon ion spectra using gases pulsed electrical discharges [40–43] (and references therein). We used experimental data of the xenon spectrum covering the wavelength range 230 – 7000 Å for the UV-Visible region. A set of 40 transitions of Xe VII and 25 transitions of Xe VIII were classified for the first time. We revised the values for the previously known energy levels and extended the analysis for Xe VII to 10 new energy levels belonging to $5s6d$, $5s7s$ and $5s7p$ $4d^95s^25p$ even and odd configurations, respectively. 7 new energy levels of the $4d^95s5d$ core excited configuration of Xe VIII are presented. Theoretical predictions of the configuration structure were obtained from the computer code developed by Cowan [44], which provides atomic parameters by means of Hartree–Fock relativistic (HFR) approximation. The energy matrix was calculated using energy parameters adjusted to fit the experimental energy levels.

2. Experiment

The light source used in this work was a capillary discharge experimental set built at CIOp [40], consisting of a Pyrex tube of 100 cm long and inner diameter of 0.5 cm, in which the gas excitation was produced by discharging a bank of low-inductance capacitors ranging from 20 to 280 nF, charged with voltages up to 20 kV. In the wavelength range below 2000 Å, light radiation emitted axially was analyzed using a 3 m normal incidence vacuum spectrograph with a concave diffraction grating of 1200 lines mm^{-1} . The plate factor in the first order was 2.77Å mm^{-1} . C, N, O and known

lines of xenon served as internal wavelength standards. The wavelength range above 2000 Å was recorded on a 3.4 m Ebert plane-grating spectrograph, with a diffraction grating of 600 lines mm⁻¹. The plate factor was 5.0 Å mm⁻¹ in the first order. The spectra were recorded in the first, second, and third diffraction orders. Th²³² lines from an electrodeless discharge were superimposed on the spectrograms and served as reference [45]. The positions of the observed Xe VII and Xe VIII spectral lines were determined by means of a rotating prism photoelectric semiautomatic Grant comparator. For sharp lines, the settings were reproducible within $\pm 1 \mu\text{m}$. The uncertainty in the determination of the wavelength of unperturbed lines was estimated to be $\pm 0.02 \text{ Å}$ for the VUV region and $\pm 0.01 \text{ Å}$ for the visible region. The intensity figures are visual estimates of photographic density, and are on a uniform scale only within limited wavelength ranges. To distinguish among different states of ionization, we studied the behavior of the spectral line intensity as a function of pressure.

3. Results and discussions

For the theoretical predictions and interpretation of these spectra Cowan's code [44] was used. These theoretical values were obtained by diagonalizing the energy matrices with adjusted radial parameters that minimized the discrepancies between the eigenvalues and the available experimental energies. In this work we present a revised and extended analysis for the 5s6d, 5s7s and 5s7p, 4d⁹5s²5p even and odd configurations of Xe VII and for the 4d⁹5s5d configuration of Xe VIII. The configuration sets used were 5s², 5p², 5s(5d+6d+7d+8d), 5s(6s+7s), 5p(4f+5f), 5p6p, 4f², 5d², 4d⁹5s²5d, 4d⁹5s²6s and 5s(5p+6p+7p), 5s(4f+5f), 6s4f, 5p(5d+6s), 4f5d, 4d⁹5s²5p, 4d⁹5s²4f for the Xe VII even and odd parities respectively, and 5s-10s, 5d-10d, 5g-10g, 7i-10i, 4d⁹5s², 4d⁹5s5d, 4d⁹5p² and 5p-10p, 4f-10f, 6h-10h, 8k-10k, 4d⁹5s5p, 4d⁹4f5s, 4d⁹5p5d for Xe VIII even and odd parities. Table 1 shows the new and adjusted energy level values for these ions. These values were determined in an iterative procedure where the wavenumbers of the observed lines were weighted according to their estimated uncertainties. All level designations in the table are in LS notation. We also present the percentage composition of the levels. The uncertainties of the adjusted experimental energy level values were generally less than 2 cm⁻¹. Table 2 shows the new classified lines for Xe VII and Xe VIII. The values of σ_{obs} and σ_{cal} in this table are the observed and calculated Ritz wavenumbers respectively. The difference between these values is in accordance with the uncertainty in the determination of the wavelength. In our analysis we also calculated the oscillator strengths gf and transition probabilities gA (the latter shown in Table 2), in order to compare with the experimental intensity of the new observed lines.

We adjusted the energy level values reported by Wang et al. [25] (compiled by Saloman [38]) for ³D_{1,2,3} of 5s6d and ³S₁ of 5s7s configurations. We reported new energy level values for ¹D₂ of 5s6d, ¹S₀ of 5s7s, ¹P₁ of 5s7p configurations and 7 new energy level values for 4d⁹5s²5p configuration of Xe VII spectrum.

We presented 7 new energy level values for the 4d⁹5s5d core excited configuration of Xe VIII and classified 25 new transitions with the previously known 4d⁹5s5p configuration [32].

The calculated energy level values were obtained by the least squares fit [44]. In this process, the Slater parameters were fitted to the experimental energy level, which should improve the wave function composition as well as the energy separations between the levels. Our calculations included all the energy levels experimentally known. The least squares calculation results are shown in Tables 3, 4, 5 and 6 for the Xe VII and Xe VIII. In Tables 3 and 4 we show the radial parameters for the even and odd-parity configurations of Xe VII. Similar calculations were given by Churilov et al. [28]. In Table 3 the adjusted parameters that were let free are in good agreement with the scaled Hartree–Fock (HF) values. In Table 4 the $G^3(4d, 5p)$ integral for the $4d^9 5s^2 5p$ configuration was fixed at 100% of its HF value because there are values of energy levels that are unknown. We also observed strong configuration interaction between $5s5p$ – $5p5d$ and $5s5f$ – $5p5d$ configurations that were fixed at 75% and 100% of their HF values respectively. In Table 5 we show the even parameters for Xe VIII ion, where six of the nine parameters of the $4d^9 5s5d$ configuration were let free in the calculation, because there are only 7 new experimental energy levels of the 34 levels belonging to this configuration. The other 3 energy parameters $G^0(4d,5d)$, $G^2(4d,5d)$, $G^4(4d,5d)$ were fixed and scaled to 85% of its HF values in order to reduce the standard deviation. All the configuration-interaction integrals were also scaled at 85% of their Hartree–Fock (HF) values. Table 6 shows the radial parameter values corresponding to the odd parity configurations. In this table the ζ_{4d} and $G^3(4d,5p)$ parameters corresponding to the $4d^9 5s5p$ configuration were fixed because there are values of energy levels that are unknown.

In the energy adjustment of the Xe VII the standard deviation was 175 cm^{-1} and 281 cm^{-1} for the even and odd parity. For even parity 29 free levels and 20 adjusted parameters were used. In a similar way 47 free levels and 27 adjusted parameters were used for odd parity. The standard deviation was 220 cm^{-1} and 248 cm^{-1} for the even and odd parity in Xe VIII. In this case 35 free levels and 28 adjusted parameters for even parity and 40 free levels and 28 adjusted parameters for odd parity were used.

4. Conclusions

In this work we studied the Xe VII and Xe VIII spectra covering the wavelength range 230–7000 Å for the UV-Visible region using a pulsed electrical discharges. A set of 40 transitions of Xe VII and 25 transitions of Xe VIII were classified. We revised the values for the previously known energy levels and extended the analysis for Xe VII to 10 new energy levels and 4 adjusted values belonging to $5s6d$, $5s7s$, $5s7p$, $4d^9 5s^2 5p$ configurations. 7 new energy levels of $4d^9 5s5d$ configuration of Xe VIII were presented. Relativistic Hartree–Fock calculations were used. Least-squares-fitted parametric calculations have been carried out to interpret the observed spectrum.

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Table 1 New and adjusted Xe VII and Xe VIII energy levels

XeVII	Configuration	Term	J	Exp Level (cm ⁻¹)	Fitted ^(a) (cm ⁻¹)	Composition ^(b)	Comment
	5s6d	³ D	1	475 997	475964	98	Adjusted
			2	476 250	476301	98	Adjusted
			3	476 785	476767	99	Adjusted
		¹ D	2	480 945	480941	94	New
	5s7s	³ S	1	506 258	506258	99	Adjusted
		¹ S	0	510325	510325	97	New
	5s7p	¹ P ^o	1	531 864	531536	86 5s7p ¹ P + 9 5s7p ³ P	New
	4d ⁹ 5s ² 5p	³ P ^o	1	529410	529502	73 4d ⁹ 5s ² 5p ³ P + 15 4d ⁹ 5s ² 5p ³ D + 8 5s7p ³ P	New
			2	514393	514179	80 4d ⁹ 5s ² 5p ³ P + 15 4d ⁹ 5s ² 5p ³ D	New
		³ D ^o	2	552 449	552378	58 4d ⁹ 5s ² 5p ³ D + 29 4d ⁹ 5s ² 5p ¹ D + 9 4d ⁹ 5s ² 5p ³ F	New
			3	539708	539287	72 4d ⁹ 5s ² 5p ³ D + 28 4d ⁹ 5s ² 5p ¹ F	New
		³ F ^o	3	517693	517747	55 4d ⁹ 5s ² 5p ³ F + 33 4d ⁹ 5s ² 5p ¹ F + 12 4d ⁹ 5s ² 5p ³ D	New
			4	530874	531027	100	New
		¹ D ^o	2	536687	537132	66 4d ⁹ 5s ² 5p ¹ D + 20 4d ⁹ 5s ² 5p ³ D + 12 4d ⁹ 5s ² 5p ³ P	New

Xe VIII	$4d^9 5s 5d \ (^3D)$	^4P	$5/2$	749456	749568	$65 \ 4d^9 5s 5d \ ^4P + 32 \ 4d^9 5s 5d \ ^4D$	New
	(^3D)	^4F	$5/2$	755624	755510	$29 \ 4d^9 5s 5d \ ^4F + 18 \ 4d^9 5s 5d \ ^4D + 16 \ 4d^9 5s 5d \ ^4G$	New
	(^3D)	^4P	$1/2$	757388	757364	$45 \ 4d^9 5s 5d \ ^4P + 19 \ 4d^9 5s 5d \ (^1D) \ ^2P + 14 \ 4d^9 5s 5d \ ^2P$	New
	(^3D)	^4D	$1/2$	767993	767718	$58 \ 4d^9 5s 5d \ ^4D + 17 \ 4d^9 5s 5d \ ^2P + 12 \ 4d^9 5s 5d \ (^1D) \ ^2P$	New
	(^3D)	^4D	$3/2$	769280	769547	$47 \ 4d^9 5s 5d \ ^4D + 16 \ 4d^9 5s 5d \ ^4F + 10 \ 4d^9 5s 5d \ (^1D) \ ^2D$	New
	(^1D)	^2S	$1/2$	769667	769705	$48 \ 4d^9 5s 5d \ (^1D) \ ^2S + 17 \ 4d^9 5s 5d \ (^1D) \ ^2P + 10 \ 4d^9 5s 5d \ ^2S$	New
	(^3D)	^2P	$1/2$	788973	788972	$47 \ 4d^9 5s 5d \ ^2P + 25 \ 4d^9 5s 5d \ (^1D) \ ^2P + 13 \ 4d^9 5s 5d \ (^1D) \ ^2S$	New

^aCalculated energy level values obtained using the fitted energy parameters

^bPercentages below 5% have been omitted

Table2 New classified lines of Xe VII and Xe VIII

Ion	Rel.	Observed Wavelength Vac (Å)	Wavenumber (cm-1)		Lower Level Conf. Term, J			Upper Level Conf. Term, J			gA(s ⁻¹)
	Int.		σ _{obs}	σ _{cal}							
VII	1	427.96	233667	233677	4f5s	³ F	2	5s7s	³ S	1	3.58 x 10 ⁶
VII	1	445.81	224311	224322	5s5d	¹ D	2	5s7p	¹ P	1	5.60 x 10 ⁹
VII	6	489.74	204190	204204	4f5s	³ F	2	5s6d	³ D	3	1.04 x 10 ⁶
VII	3	490.96	203683	203669	4f5s	³ F	2	5s6d	³ D	2	2.77 x 10 ⁷
VII	4	587.54	217001	216193	5s6s	¹ S	0	5s7p	¹ P	1	5.62 x 10 ⁷
VII	1	603.74	165634	165638	4f5p	³ F	2	4d ⁹ 5s ² 5p	³ D	2	6.65 x 10 ⁵
VII	4	647.61	154414	154422	4f5p	¹ F	3	4d ⁹ 5s ² 5p	³ D	2	1.26 x 10 ³
VII	3	654.02	152901	152897	4f5p	³ F	2	4d ⁹ 5s ² 5p	³ D	3	3.24 x 10 ⁴
VII	3	661.09	151265	151265	4f5p	³ F	3	4d ⁹ 5s ² 5p	¹ D	2	4.41 x 10 ⁵
VII	4	673.35	148511	148518	4f5p	³ G	3	4d ⁹ 5s ² 5p	³ F	4	3.48 x 10 ⁴
VII	5	687.53	145448	145452	4f5p	³ F	3	4d ⁹ 5s ² 5p	³ F	4	4.42 x 10 ⁶
VII	4	715.70	139723	139721	4f5p	³ F	4	4d ⁹ 5s ² 5p	³ D	3	1.21 x 10 ⁶
VII	5	721.19	138660	138660	4f5p	¹ F	3	4d ⁹ 5s ² 5p	¹ D	2	1.51 x 10 ⁶

VII	5	734.83	136086	136092	4f5p	¹ D	2	4d ⁹ 5s ² 5p	³ D	2	3.22 x 10 ⁷
VII	2	742.23	134729	134729	4f5p	³ D	3	4d ⁹ 5s ² 5p	³ D	3	1.65 x 10 ⁶
VII	5	756.03	132270	132271	4f5p	³ F	3	4d ⁹ 5s ² 5p	³ F	3	3.66 x 10 ⁶
VII	7	764.02	130887	130882	4f5p	³ F	2	4d ⁹ 5s ² 5p	³ F	3	2.61 x 10 ⁷
VII	7	764.02	130887	130887	4f5p	³ F	4	4d ⁹ 5s ² 5p	³ F	4	2.10 x 10 ⁷
VII	1	775.37	128971	128971	4f5p	³ F	3	4d ⁹ 5s ² 5p	³ P	2	5.49 x 10 ⁶
VII	5	781.76	127917	127920	4f5p	³ D	1	4d ⁹ 5s ² 5p	¹ D	2	2.69 x 10 ⁴
VII	2	812.56	123068	123068	4f5p	³ D	2	4d ⁹ 5s ² 5p	³ P	1	3.29 x 10 ⁶
VII	5	828.91	120640	120643	4f5p	³ D	1	4d ⁹ 5s ² 5p	³ P	1	1.91 x 10 ⁶
VII	3	831.03	120333	120330	4f5p	¹ D	2	4d ⁹ 5s ² 5p	¹ D	2	1.44 x 10 ⁵
VII	5	859.33	116370	116366	4f5p	¹ F	3	4d ⁹ 5s ² 5p	³ P	2	2.07 x 10 ⁵
VII	4	884.51	113057	113053	4f5p	¹ D	2	4d ⁹ 5s ² 5p	³ P	1	2.17 x 10 ⁶
VII	6	887.20	112714	112714	4f5p	³ D	3	4d ⁹ 5s ² 5p	³ F	3	1.69 x 10 ⁶
VII	8	898.03	111355	111351	4f5p	³ D	2	4d ⁹ 5s ² 5p	³ F	3	6.41 x 10 ⁵
VII	7	925.51	108049	108051	4f5p	³ D	2	4d ⁹ 5s ² 5p	³ P	2	8.63 x 10 ⁵
VII	7	942.16	106139	106142	4f5p	¹ G	4	4d ⁹ 5s ² 5p	³ F	3	3.76 x 10 ⁸
VII	1	947.05	105591	105592	5s6p	³ P	0	5s7s	³ S	1	3.20 x 10 ⁹
VII	4	975.38	102524	102523	5s6p	¹ P	1	5s7s	¹ S	0	2.73 x 10 ⁹

VII	4	1212.73	82459	82458	5p5d	³ F	2	5s6d	³ D	2	1.36 x 10 ⁸
VII	7	1234.17	81026	81024	5p5d	³ P	2	5s7s	³ S	1	1.84 x 10 ⁸
VII	1	1321.64	75664	75663	5s6d	³ D	3	4d ⁹ 5s ² 5p	³ D	2	4.28 x 10 ⁵
VII	2	1460.95	68449	68448	5s6p	¹ P	1	5s6d	³ D	2	1.18 x 10 ⁹
VII	2	1539.03	64976	64975	5p5d	³ D	1	5s6d	³ D	1	1.16 x 10 ⁸
VII	1	1541.24	64883	64882	5p5d	¹ P	1	5s7s	³ S	1	3.96 x 10 ⁶
VII	7	1557.13	64221	64218	5p5d	³ F	4	5s6d	³ D	3	9.51 x 10 ⁸
VII	7	1726.57	57918	57917	5p5d	³ D	3	5s6d	¹ D	2	1.27 x 10 ⁸
VII	7	1963.86	50920	50919	5s6d	¹ D	2	5s7p	¹ P	1	3.44 x 10 ⁹
VII	9	4641.31	21540	21539	5s7s	¹ S	0	5s7p	¹ P	1	2.45 x 10 ⁸
		Observed Wavelength Vac (Å)									
VIII	8	419.22	238538	238524	4d ⁹ 5s5p	⁴ F	3/2	4d ⁹ 5s5d	(³ D) ² P	1/2	4.55 x 10 ⁸
VIII	2	430.34	232374	232364	4d ⁹ 5s5p	(¹ D) ² D	3/2	4d ⁹ 5s5d	(³ D) ² P	1/2	1.05 x 10 ¹⁰
VIII	1	439.13	227723	227725	4d ⁹ 5s5p	⁴ P	3/2	4d ⁹ 5s5d	⁴ D	3/2	2.67 x 10 ¹⁰
VIII	1	441.62	226439	226438	4d ⁹ 5s5p	⁴ P	3/2	4d ⁹ 5s5d	⁴ D	1/2	2.24 x 10 ⁹
VIII	4	444.78	224830	224824	4d ⁹ 5s5p	(¹ D) ² P	1/2	4d ⁹ 5s5d	(³ D) ² P	1/2	3.96 x 10 ⁸

VIII	4	459.70	217533	217544	$4d^9 5s 5p$	^4F	3/2	$4d^9 5s 5d$	^4D	1/2	2.70×10^9
VIII	1	463.32	215834	215833	$4d^9 5s 5p$	^4P	3/2	$4d^9 5s 5d$	^4P	1/2	3.80×10^{10}
VIII	2	470.23	212662	212671	$4d^9 5s 5p$	$(^1D)^2D$	3/2	$4d^9 5s 5d$	^4D	3/2	1.30×10^9
VIII	4	473.05	211394	211384	$4d^9 5s 5p$	$(^1D)^2D$	3/2	$4d^9 5s 5d$	^4D	1/2	1.42×10^9
VIII	2b1	480.98	207909	207901	$4d^9 5s 5p$	^4P	3/2	$4d^9 5s 5d$	^4P	5/2	1.32×10^9
VIII	3	483.22	206945	206939	$4d^9 5s 5p$	^4F	3/2	$4d^9 5s 5d$	^4P	1/2	1.27×10^9
VIII	3	483.22	206945	206937	$4d^9 5s 5p$	$(^1D)^2P$	3/2	$4d^9 5s 5d$	$(^1D)^2S$	1/2	7.27×10^9
VIII	4	487.40	205170	205175	$4d^9 5s 5p$	^4F	3/2	$4d^9 5s 5d$	^4F	5/2	2.00×10^7
VIII	3	490.96	203683	203685	$4d^9 5s 5p$	$(^3D)^2P$	3/2	$4d^9 5s 5d$	$(^3D)^2P$	1/2	1.07×10^{10}
VIII	1	497.31	201082	201072	$4d^9 5s 5p$	^4D	1/2	$4d^9 5s 5d$	$(^1D)^2S$	1/2	3.05×10^7
VIII	4	498.04	200787	200779	$4d^9 5s 5p$	$(^1D)^2D$	3/2	$4d^9 5s 5d$	^4P	1/2	1.06×10^8
VIII	2	501.51	199398	199398	$4d^9 5s 5p$	^4D	1/2	$4d^9 5s 5d$	^4D	1/2	1.86×10^9
VIII	7	502.50	199005	199007	$4d^9 5s 5p$	^4F	3/2	$4d^9 5s 5d$	^4P	5/2	2.78×10^8
VIII	7	502.50	199005	199015	$4d^9 5s 5p$	$(^1D)^2D$	3/2	$4d^9 5s 5d$	^4F	5/2	2.00×10^{10}
VIII	2	512.68	195053	195052	$4d^9 5s 5p$	^4D	3/2	$4d^9 5s 5d$	^4D	3/2	3.41×10^8
VIII	4	513.69	194670	194658	$4d^9 5s 5p$	$(^1D)^2P$	3/2	$4d^9 5s 5d$	^4P	1/2	4.21×10^7
VIII	1	517.49	193241	193239	$4d^9 5s 5p$	$(^1D)^2P$	1/2	$4d^9 5s 5d$	^4P	1/2	2.10×10^9
VIII	2	542.36	184379	184379	$4d^9 5s 5p$	$(^3D)^2P$	3/2	$4d^9 5s 5d$	$(^1D)^2S$	1/2	2.14×10^{10}

VIII	6	547.35	182698	182705	$4d^9 5s 5p$	$(^3D)^2P$	3/2	$4d^9 5s 5d$	^4D	1/2	4.26×10^9
VIII	2	551.27	181399	181396	$4d^9 5s 5p$	^4D	3/2	$4d^9 5s 5d$	^4F	5/2	1.33×10^{10}
VIII	6	1614.37	61944	61944	$4d^9 5s 5d$	^4P	5/2	$4d^9 5s 4f$	^2P	3/2	5.22×10^8

Note: bl, blended line

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

Configuration	Parameter	H-F value	Fitted value	Fitt/H-F ^a
5s ²	E _{av}	0	7009 ± 174	
5p ²	E _{av}	238023	248510 ± 143	1.04
	F ² (5p, 5p)	59078	53119 ± 1789	0.90
	α	0	545 (FIX)	
	ζ _{5p}	10548	11632 ± 93	1.10
5s5d	E _{av}	283684	293214 ± 97	1.03
	ζ _{5d}	842	1064 ± 95	1.26
	G ² (5s,5d)	38699	26141 ± 655	0.68
5s6d	E _{av}	467624	478435 ± 90	0.98
	ζ _{6d}	377	358	0.95
	G ² (5s,6d)	9108	11945 ± 527	1.31
5s7d	E _{av}	555672	555672 (FIX)	1.00
5s8d	E _{av}	605411	605411 (FIX)	1.00
5s6s	E _{av}	347141	358325 ± 135	1.03
	G ⁰ (5s, 6s)	5194	4160 ± 121	0.80
5s7s	E _{av}	494169	507618 ± 135	1.03
	G ⁰ (5s, 7s)	1789	2464 ± 122	1.40
4f5p	E _{av}	388140	398510 ± 50	1.03
	ζ _{4f}	254	202 ± 36	0.80
	ζ _{5p}	10135	11505 ± 97	1.14
	F ² (4f, 5p)	51181	42077 ± 621	0.82
	G ² (4f, 5p)	35098	29717 ± 441	0.85
	G ⁴ (4f, 5p)	26034	19416 ± 635	0.75
5f5p	E _{av}	577384	577384 (FIX)	1.00
5p6p	E _{av}	521670	521670 (FIX)	1.00
4f ²	E _{av}	546646	546646 (FIX)	1.00
5d ²	E _{av}	581986	581986 (FIX)	1.00
5s ² 5d	E _{av}	721545	721545 (FIX)	1.00

5s ² 6s	E _{av}	788768	788768 (FIX)	1.00
^a Parameters omitted from this table: direct and exchange integrals, and spin-orbit ζ parameters set to 85% and 95% of their HFR values respectively; CI integrals were set to 85% of their HFR values. The standard deviation for the energy adjustment was 175 cm ⁻¹ .				

Table 4 Energy parameters (cm⁻¹) for the studied odd parity configurations of Xe VII

Configuration	Parameter	H-F value	Fitted value	Fitt/H-F ^a
5s5p	E _{av}	108319	118939 ± 154	1.10
	ζ_{5p}	10622	11694 ± 246	1.10
	G ¹ (5s,5p)	76747	62102 ± 579	0.81
5s6p	E _{av}	396097	407212 ± 92	1.03
	ζ_{6p}	3931	4626 ± 260	1.17
	G ¹ (5s,6p)	8539	6315 ± 903	0.74
5s7p	E _{av}	518483	529156 ± 161	1.02
	ζ_{7p}	1975	1593 ± 221	0.81
	G ¹ (5s,7p)	3176	2699(FIX)	0.85
5s4f	E _{av}	268592	275519 ± 144	1.03
	ζ_{4f}	245	233 (FIX)	0.95
	G ³ (5s,4f)	36153	29814 ± 1172	0.82
6s4f	E _{av}	615059	615059 (FIX)	1.00
	ζ_{4f}	271	258 (FIX)	0.95
	G ³ (6s,4f)	6425	5461 (FIX)	0.85
5s5f	E _{av}	452423	461307 ± 154	1.02
	ζ_{5f}	87	87 (FIX)	1.00
	G ³ (5s,5f)	4396	4854 ± 1391	1.10
5p5d	E _{av}	406352	418416 ± 95	1.03
	ζ_{5p}	10741	11387 ± 239	1.06
	ζ_{5d}	861	1495 ± 151	1.73
	F ² (5p, 5d)	49703	39181 ± 1042	0.79
	G ¹ (5p, 5d)	58495	43670 ± 503	0.73

	$G^3(5p, 5d)$	37389	27187 ± 1042	0.73
5p6s	E_{av}	473884	480754 ± 154	1.01
	ζ_{5p}	11075	11175 ± 221	1.01
	$G^1(5p, 6s)$	7801	7627 ± 750	0.98
4f5d	E_{av}	552712	552712 (FIX)	1.00
$4d^9 5s^2 5p$	E_{av}	532109	534424 ± 105	1.01
	ζ_{4d}	6274	5497 ± 119	0.88
	ζ_{5p}	11481	10924 ± 230	0.95
	$F^2(4d, 5p)$	41900	37782 ± 1146	0.90
	$G^1(4d, 5p)$	12567	11261 ± 334	0.90
	$G^3(4d, 5p)$	12260	12260 (FIX)	1.00
$4d^9 5s^2 4f$	E_{av}	684316	659204 ± 284	0.96
Configuration Interaction Integrals				
5s5p – 5p5d	$R^1(5s5p, 5p5d)$	65548	49167 (FIX)	0.75
5s5p – 5p5d	$R^2(5p5d, 5s5p)$	48216	36167 (FIX)	0.75
5s5f – 5p5d	$R^1(5s5f, 5p5d)$	28688	28688 (FIX)	1.00

^a Parameters omitted from this table: direct and exchange integrals, and spin-orbit ζ parameters set to 85% and 95% of their HFR values respectively; CI integrals were set to 85% of their HFR values. The standard deviation for the energy adjustment was 281 cm^{-1} .

Table 5 Energy parameters (cm^{-1}) for the studied even parity configurations of Xe VIII

Configuration	Parameter	H-F value	Fitted value	Fitt/H-F ^a
5s	E_{av}	0	1604 ± 221	
6s	E_{av}	390824	395674 ± 220	1.01
7s	E_{av}	559648	565446 ± 220	1.01
8s	E_{av}	648997	655344 ± 221	1.01
9s	E_{av}	702240	708802 ± 221	1.01
10s	E_{av}	738183	738183 (FIX)	1.00
5d	E_{av}	307328	311934 ± 159	1.01
	ζ_{5d}	973	1166 ± 125	1.20

6d	E_{av}	523083	528291±159	1.01
	ζ_{6d}	458	544±125	1.19
7d	E_{av}	629182	635100±159	1.01
	ζ_{7d}	254	302±125	1.19
8d	E_{av}	690206	696750±170	1.01
	ζ_{8d}	156	148 (FIX)	0.95
9d	E_{av}	728695	735363±158	1.01
	ζ_{9d}	102	97 (FIX)	0.95
10d	E_{av}	756178	756178 (FIX)	1.00
	ζ_{10d}	72	68 (FIX)	0.95
5g	E_{av}	563128	570278±156	1.01
6g	E_{av}	650133	656870±156	1.01
7g	E_{av}	702603	709348±156	1.01
8g	E_{av}	736661	743659±222	1.01
9g	E_{av}	760007	767020±236	1.01
10g	E_{av}	776700	778305 (FIX)	1.01
7i	E_{av}	704151	711319±220	1.01
8i	E_{av}	737746	744899±220	1.01
9i	E_{av}	760797	767987±220	1.01
10i	E_{av}	777285	784500±220	1.01
$4d^9 5s^2$	E_{av}	450587	450587 (FIX)	1.00
$4d^9 5s 5d$	E_{av}	759876	763956±173	1.01
	ζ_{4d}	6369	6544±114	1.03
	ζ_{5d}	1047	995 (FIX)	0.95
	$F^2(4d, 5d)$	30132	33655±2018	1.12
	$F^4(4d, 5d)$	14001	13887±1997	0.99
	$G^2(4d, 5s)$	18389	20662±3193	1.12
	$G^0(4d, 5d)$	7059	6000 (FIX)	0.85
	$G^2(4d, 5d)$	8874	7543 (FIX)	0.85
	$G^4(4d, 5d)$	7433	6318 (FIX)	0.85

	$G^2(5s,5d)$	42987	33247 ± 1470	0.77
$4d^9 5p^2$	E_{av}	708344	708344 (FIX)	

^a Parameters omitted from this table: direct and exchange integrals, and spin-orbit ζ parameters set to 85% and 95% of their HFR values respectively; CI integrals were set to 85% of their HFR values. The standard deviation for the energy adjustment was 220 cm^{-1} .

Table 6 Energy parameters (cm^{-1}) for the studied odd parity configurations of Xe VIII

Configuration	Parameter	H-F value	Fitted value	Fitt/H-F ^a
5p	E_{av}	127266	133349 ± 186	1.05
	ζ_{5p}	11381	12447 ± 235	1.09
6p	E_{av}	443669	449194 ± 185	1.01
	ζ_{6p}	4650	4933 ± 235	1.06
7p	E_{av}	586793	593045 ± 179	1.01
	ζ_{7p}	2395	2275 (FIX)	0.95
8p	E_{av}	664825	671726 ± 176	1.01
	ζ_{8p}	1403	1333 (FIX)	0.95
9p	E_{av}	712278	719104 ± 186	1.01
	ζ_{9p}	894	922 ± 235	1.03
10p	E_{av}	743345	743345 (FIX)	1.00
4f	E_{av}	263400	265561 ± 176	1.01
	ζ_{4f}	282	268 (FIX)	0.95
5f	E_{av}	493775	497866 ± 175	1.01
	ζ_{5f}	105	100 (FIX)	0.95
6f	E_{av}	611494	616577 ± 176	1.01
	ζ_{6f}	55	52 (FIX)	0.95
7f	E_{av}	678916	684573 ± 176	1.01
	ζ_{7f}	33	31 (FIX)	0.95
8f	E_{av}	721106	727379 ± 175	1.01
	ζ_{8f}	21	20 (FIX)	0.95

9f	E_{av}	749252	755759 ± 175	1.01
	ζ_{9f}	15	14 (FIX)	0.95
10f	E_{av}	768949	768949 (FIX)	1.00
6h	E_{av}	651951	659192 ± 176	1.01
7h	E_{av}	703834	711059 ± 248	1.01
8h	E_{av}	737538	744772 ± 248	1.01
9h	E_{av}	760653	767888 ± 248	1.01
10h	E_{av}	777184	777184 (FIX)	1.00
8k	E_{av}	737816	744951 ± 248	1.01
9k	E_{av}	760848	767985 ± 248	1.01
10k	E_{av}	777325	784478 ± 248	1.01
4d ⁹ 5s5p	E_{av}	566334	567120 ± 162	1.01
	ζ_{4d}	6342	6025 (FIX)	0.95
	ζ_{5p}	12229	14224 ± 280	1.16
	$F^2(4d, 5p)$	43498	35529 ± 2304	0.82
	$G^2(4d, 5s)$	18331	19275 ± 1771	1.05
	$G^1(4d, 5p)$	13040	11665 ± 479	0.89
	$G^3(4d, 5p)$	12788	10870 (FIX)	0.85
	$G^1(5s, 5p)$	80420	56775 ± 702	0.71
4d ⁹ 4f5s	E_{av}	693106	651800 ± 180	0.94
4d ⁹ 5p5d	E_{av}	891877	891877 (FIX)	1.00

^a Parameters omitted from this table: direct and exchange integrals, and spin-orbit ζ parameters set to 85% and 95% of their HFR values respectively; CI integrals were set to 85% of their HFR values. The standard deviation for the energy adjustment was 248 cm^{-1} .