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New energy levels, calculated lifetimes and transition probabilities in Xe IX

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Abstract
Twenty-one new experimental energy levels belonging to the $4d^96p$, $4d^94f$ and $4d^95f$ configurations of Xe IX are presented. They have been deduced from 75 newly classified lines involving the configurations $4d^95p$, $4d^96p$, $4d^94f$, $4d^95f$ and $4d^95d$, $4d^95s$, $4d^96s$ for the odd and even parities, respectively. The radiative lifetimes of these levels as well as the weighted oscillator strengths and transition probabilities for all the observed spectral lines have been calculated with optimized parameters deduced from a least-squares fitting procedure applied in the framework of a relativistic Hartree–Fock method including core-polarization effects. The scale of transition probabilities has also been assessed through comparisons with lifetimes calculated using a relativistic multiconfigurational Dirac–Fock approach.

1. Introduction

Spectroscopic data on rare gases are needed in relation to fusion diagnostics, laser physics, photoelectron spectroscopy and collision physics. Radiative parameters for high members of the Pd I isoelectronic sequence are important for achieving laser action at short wavelengths, and this effect has been demonstrated for Xe IX at the wavelength of 418.1 Å [1].

Previous investigations of the Xe^{8+} spectrum and of the transition probabilities in this ion are still rather scarce. Resonance transitions involving the $4d^9(np + nf)$ configurations were studied along the Pd I isoelectronic sequence, from Cd III to Cs X, by Churilov *et al* [2, 3]. The spectra of Cd III, In IV and Sn V were investigated by Joshi and van Kleef [4, 5], and the previous studies on Sb VI, Te VII, I VIII and Xe IX [6], were revised and extended by Churilov *et al* [7–9]. The analysis of the Cs X–Ce XIII, and Pr XIV–Nd XV spectra has been published by Churilov *et al* [10, 11]. Recently, a compilation of energy levels and observed lines of xenon ions, from Xe I to Xe LIV, was reported by Saloman [13] and the analysis of the $4d^96s$ configuration in eight times ionized xenon was published by Raineri *et al* [14].

The previous work on transition probabilities or lifetimes includes the calculations in the ions Xe IX to Ce XIII performed by Loginov [12]. Calculations of oscillator strengths and transition probabilities in Pd-like ions were also reported by Safranova *et al* [15] and a similar approach was used to obtain wavelengths, transition rates and line strengths along the same sequence [16]. A new set of lifetimes and transition probabilities in Xe IX was recently reported by Garnir *et al* [17] and experimental and theoretical studies related to the laser action in Xe IX are due to Reyna Almandos *et al* [18].

Palladium-like xenon, Xe IX, has a closed $4d^{10}$ shell in its ground state. The present investigation aims at extending our knowledge of the Xe^{8+} ion concerning both the term analysis and the radiative parameter determination. More precisely, we have studied the $4d^96p$, $4d^94f$ and $4d^95f$ configurations of Xe IX. New energy levels belonging to these configurations have been determined using transitions emitted from the previously known $4d^95d$ and $4d^96s$ configurations. New observed lines, classified as $4d^95p$–$4d^95d$ and $4d^95s$–$4d^95p$ transitions, are also reported. The present spectral analysis was supported by theoretical calculations using Cowan's codes [19] and by fitting the calculated eigenvalues of the Hamiltonian to the experimental energy levels belonging to the $4d^96p$, $4d^94f$ and $4d^95f$ configurations along the Pd I sequence. The relativistic Hartree–Fock (HFR) calculations of lifetimes and transition probabilities were compared to the multiconfiguration Dirac–Fock (MCDF) results [20, 21]. The effects of core-polarization effects on the calculated lifetimes and transition probabilities have also been investigated using a modified version of Cowan's computer codes [22, 23].

Table 1. Experimental and calculated energy levels and their percentage composition for the $4d^96p$ and $4d^95f$ configurations of Xe IX. Calculated radiative lifetimes, τ (ns), are also given. For all the transitions, the core is $4d^9$.

Level	$E_{\mathrm{Experimental}}$ (cm^{-1})	$E_{\mathrm{Calculated}}$[a] (cm^{-1})	Composition (%)[b]	τ (ns) HFR(A)[e]	HFR(B)[f]	GRASP[g]
$4d^96p\ ^3P^\circ_2$	954 480[n]	954 211	72 6p $^3P^\circ$, 22 6p $^3D^\circ$, 5 6p $^1D^\circ$	0.0708	0.0655	0.0663
$^3F^\circ_3$	955 120[n]	955 200	49 6p $^3F^\circ$, 36 6p $^1F^\circ$, 14 6p $^3D^\circ$	0.0710	0.0658	0.0650
$^3F^\circ_4$	962 302[n]	962 373	100 6p $^3F^\circ$	0.0644	0.0597	0.0733
$^3P^\circ_1$	963 316[c]	963 534	48 6p $^3P^\circ$, 41 6p $^1P^\circ$, 10 6p $^3D^\circ$	0.0227	0.0275	0.0686
$^1D^\circ_2$		963 845	46 6p $^1D^\circ$, 22 6p $^3P^\circ$, 20 6p $^3D^\circ$	0.0656	0.0612	0.0768
$^3D^\circ_3$	965 365[n]	965 272	77 6p $^3D^\circ$, 23 6p $^1F^\circ$	0.0653	0.0602	0.0803
$^3F^\circ_2$	970 681[n]	971 021	75 6p $^3F^\circ$, 24 6p $^1D^\circ$	0.0724	0.0602	0.0658
$^1P^\circ_1$	972 664[c]	972 495	53 6p $^1P^\circ$, 26 6p $^3D^\circ$, 20 6p $^3P^\circ$	0.0204	0.0263	0.0613
$^3P^\circ_0$	976 750[n]	976 643	100 6p $^3P^\circ$	0.0645	0.0603	0.0727
$^3F^\circ_3$		979 321	50 6p $^3F^\circ$, 41 6p $^1F^\circ$, 9 6p $^3D^\circ$	0.0641	0.0601	0.0640
$^3D^\circ_1$		979 678	64 6p $^3D^\circ$, 31 6p $^3P^\circ$	0.0553	0.0585	0.0648
$^3D^\circ_2$	981 146[n]	981 076	58 6p $^3D^\circ$, 25 6p $^1D^\circ$, 11 6p $^3F^\circ$	0.0662	0.0608	0.0801
$4d^95f\ ^3P^\circ_0$		990 295	100 5f $^3P^\circ$	0.0370	0.0414	0.0396
$^3P^\circ_1$		991 835	88 5f $^3P^\circ$, 11 5f $^3D^\circ$	0.0352	0.0418	0.0399
$^3P^\circ_2$		994 249	62 5f $^3P^\circ$, 25 5f $^3D^\circ$, 13 $^1D^\circ$	0.0379	0.0432	0.0409
$^3H^\circ_6$	995 182[n]	995 414	100 5f $^3H^\circ$	0.0377	0.0440	0.0417
$^3H^\circ_5$	995 961[d]	995 842	54 5f $^3H^\circ$, 46 $^1H^\circ$	0.0362	0.0428	0.0413
$^3F^\circ_2$	998 024[d]	997 938	39 5f $^3F^\circ$, 38 5f $^1D^\circ$, 22 5f $^3D^\circ$	0.0372	0.0437	0.0423
$^3F^\circ_3$	998 220[d]	998 149	49 5f $^3F^\circ$, 47 5f $^3D^\circ$	0.0371	0.0436	0.0419
$^3F^\circ_4$	998 989[d]	998 911	79 5f $^3F^\circ$, 17 5f $^3G^\circ$	0.0390	0.0445	0.0428
$^1G^\circ_4$	999 794[d]	999 861	47 5f $^1G^\circ$, 28 5f $^3G^\circ$, 23 5f $^3H^\circ$	0.0367	0.0440	0.0425
$^3G^\circ_5$	1000 432[d]	1000 409	78 5f $^3G^\circ$, 15 5f $^1H^\circ$, 7 5f $^3H^\circ$	0.0379	0.0452	0.0431
$^1F^\circ_3$	1001 354[d]	1001 396	48 5f $^1F^\circ$, 21 5f $^3D^\circ$, 20 5f $^3G^\circ$	0.0377	0.0447	0.0431
$^3D^\circ_1$	1004 468[d]	1004 541	85 5f $^3D^\circ$, 10 5f $^3P^\circ$	0.0171	0.0432	0.0412
$^3D^\circ_2$	1010 983[n]	1010 845	37 5f $^3P^\circ$, 36 5f $^3D^\circ$, 27 5f $^1D^\circ$	0.0382	0.0441	0.0417
$^3H^\circ_4$	1012 122[d]	1012 287	76 5f $^3H^\circ$, 14 5f $^1G^\circ$, 10 5f $^3G^\circ$	0.0365	0.0429	0.0415
$^1H^\circ_5$	1013 161[d]	1013 307	39 5f $^1H^\circ$, 39 5f $^3H^\circ$, 21 5f $^3G^\circ$	0.0379	0.0450	0.0424
$^3F^\circ_2$	1014 147[d]	1014 225	60 5f $^3F^\circ$, 22 5f $^1D^\circ$, 17 5f $^3D^\circ$	0.0371	0.0436	0.0422
$^3F^\circ_3$	1015 439[d]	1015 600	40 5f $^3F^\circ$, 26 5f $^3D^\circ$, 23 5f $^3G^\circ$	0.0382	0.0452	0.0429
$^3G^\circ_4$	1016 855[n]	1016 850	46 5f $^3G^\circ$, 35 5f $^1G^\circ$, 19 5f $^3F^\circ$	0.0381	0.0456	0.0434
$^3G^\circ_3$	1017 705[n]	1017 612	53 5f $^3G^\circ$, 41 5f $^1F^\circ$, 7 5f $^3D^\circ$	0.0368	0.0440	0.0429
$^1P^\circ_1$	1036 788[d]	1036 784	83 5f $^3P^\circ$, 7 5f $^1P^\circ$	0.00187	0.0552	0.0335

[a] Calculated values of this work.
[b] Percentages below 5% have been omitted.
[c,d] The energy level has been measured previously in [3] and [9] respectively.
[n] New energy level.
[e] HFR(A) HFR calculation: of this work (see the text).
[f] HFR(B) HFR calculation including core-polarization effects: of this work (see the text).
[g] GRASP MCDF calculation: of this work (see the text).

2. Experimental details

The light source used in this work is a discharge tube built at CIOp, adapted to the study of noble gases in the VUV region [18]. It was recently used in the cases of Ne IV [24], Ar VI [25] and Xe V [26]. It consists of a Pyrex tube of about 100 cm having an inner diameter of 0.5 cm. The electrodes, placed 80 cm apart, are made of tungsten, covered with indium to avoid the impurities coming from the electrodes. At one side of the tube there is an inlet, connected via a pressure reduction system, to the bottle of xenon. One end of the tube was connected to a vacuum spectrograph through a nylon flange adaptor and the other end had a glass window for observing the discharge. Gas excitation was produced by discharging a bank of low-inductance capacitors by quick switches (spark gap or thyratron, the latter one being used to obtain better stability in the discharge) of 200 nF and charged up to 18 kV through the tube. The pressure range was varied between 5 and 100 mTorr and the current was damped sinusoidal with a period of 2 μs, having peak values between 1 and 3.5 kA. Light radiation emitted axially was recorded between 280 and 2100 Å using a 3 m normal incidence vacuum spectrograph with a concave diffraction grating with 1200 lines mm^{-1} blazed at 1200 Å, with a plate factor of 2.77 Å mm^{-1} in the first diffraction order. The gas pressure, the discharge voltage and the capacitance were varied to distinguish the different ionization stages. To record the new spectra, Ilford Q plates were used. As internal wavelength standards, known lines of C, N, O and Xe ions were used. The spectrograms were measured with a photoelectric automatic Grant comparator whose precision is 1 μm. The uncertainty in the determination of the wavelength values of unperturbed lines presented in this work was estimated to be $\pm$0.02 Å.

Table 2. Experimental and calculated energy levels of the $4d^94f$ configuration of Xe IX. The percentage compositions are also given.

Level	$E_{Exp.}$ (cm^{-1})	$E_{Calc.}$[a] (cm^{-1})	Composition (%)[b]
$4d^94f\ ^3P^\circ_0$	663 105[n]	662 988	100 4f $^3P^\circ$
$^3P^\circ_1$	665 447[d]	665 495	98 4f $^3P^\circ$
$^3P^\circ_2$		670 478	92 4f $^3P^\circ$, 5 4f $^3D^\circ$
$^3H^\circ_6$		680 371	100 4f $^3H^\circ$
$^3H^\circ_5$		683 662	83 4f $^3H^\circ$, 16 4f $^1H^\circ$
$^3H^\circ_4$	690 894[n]	690 962	89 4f $^3H^\circ$, 6 4f $^1G^\circ$
$^1D^\circ_2$		691 330	40 4f $^1D^\circ$, 30 4f $^3D^\circ$, 29 $^3F^\circ$
$^3D^\circ_3$	692 071[n]	692 084	65 4f $^3D^\circ$, 33 4f $^3F^\circ$
$^3F^\circ_4$	695 779[n]	695 761	89 4f $^3F^\circ$, 6 4f $^3G^\circ$
$^3D^\circ_1$	696 314[d]	696 243	98 4f $^3D^\circ$
$^3D^\circ_2$	698 472[n]	698 521	52 4f $^3D^\circ$, 40 4f $^1D^\circ$, 7 4f $^3P^\circ$
$^1H^\circ_5$		698 869	62 4f $^1H^\circ$, 30 4f $^3G^\circ$, 8 4f $^3H^\circ$
$^3F^\circ_3$	701 228[n]	701 435	50 4f $^3F^\circ$, 28 4f $^3D^\circ$, 13 4f $^3G^\circ$
$^1G^\circ_4$	706 424[n]	706 307	51 4f $^1G^\circ$, 38 4f $^3G^\circ$, 11 4f $^3H^\circ$
$^3F^\circ_2$		707 164	71 4f $^3F^\circ$, 16 4f $^1D^\circ$, 13 4f $^3D^\circ$
$^3G^\circ_5$		708 354	69 4f $^3G^\circ$, 22 4f $^1H^\circ$, 9 4f $^3H^\circ$
$^3G^\circ_3$	714 354[n]	714 518	73 4f $^3G^\circ$, 16 4f $^3F^\circ$, 7 4f $^1F^\circ$
$^3G^\circ_4$	716 992[n]	716 801	50 4f $^3G^\circ$, 40 4f $^1G^\circ$, 10 4f $^3F^\circ$
$^1F^\circ_3$	724 738[n]	724 701	83 4f $^1F^\circ$, 13 4f $^3G^\circ$
$^1P^\circ_1$	832 414[d]	832 414	89 4f $^1P^\circ$, 9 5f $^1P^\circ$

[a] Calculated values of this work.
[b] Percentages below 5% have been omitted.
[d] The energy level has been measured earlier in [9].
[n] New energy level.

3. Term analysis

The new energy levels belonging to the $4d^96p$ and $4d^95f$ configurations and their percentage compositions, obtained from a least-squares fitting procedure, are shown in table 1 which also includes the calculated lifetimes (see the next section). The energy levels of the $4d^94f$ configuration, as well as their composition, are reported in table 2. In tables 3 and 4, we present 75 newly classified lines involving the configurations $4d^95p$, $4d^96p$, $4d^94f$, $4d^95f$ and $4d^95d$, $4d^95s$, $4d^96s$ for odd and even parity, respectively. The intensities of the lines were based on visual estimates deduced from the observed spectra and the calculated wavenumbers were deduced from the optimized level values. In this table, we have also included four newly observed lines, classified in the work of Garnir *et al* [17].

For the $4d^96p$ configuration, we adjusted the resonant levels published in the work of Churilov [3] and we propose seven new energy levels in this configuration. Ten new levels of the $4d^94f$ configuration and four new levels of the $4d^95f$ configuration were determined. In this last configuration, we changed the $^3G_3$ energy level value reported in [9] and we propose a new value (1017 705 cm^{-1}) established from the observation of four new transitions. This level value is in good agreement with the results obtained along the isoelectronic sequence [7, 9,11]. In [9], the $4d^95f\ ^3G^\circ_4$ energy level was determined from only one line that appears in our spectra with a very low intensity. We propose a new value of 1016 855 cm^{-1} for this level, this result being determined now from three new transitions. We also adjusted the value of the $4d^95f\ ^1G^\circ_4$ energy level and changed the $4d^95f\ ^3H^\circ_6$ level value reported by Churilov [9], this change being based on the observation of a new transition instead of using the line with double classification considered in [9].

4. Calculations of lifetimes and transition probabilities

Calculations of energy levels, lifetimes and transition probabilities in Xe IX have been carried out using the HFR approach [19], eventually modified for inclusion of core-polarization effects (HFR+CPOL approach) [22, 23].

In fact, Migdalek and Baylis [27, 28] have suggested an approach in which most of the intravalence correlation is represented within a CI scheme while the core–valence correlation for systems with more than one valence electron is described by a core-polarization model potential with a core-penetration corrective term.

Two separate calculations were performed. In the first one (hereafter designated as HFR(A)) not including the CPOL contributions, the sets of configurations retained included the $4d^{10}$, $4d^9ns$ ($n = 5, 6$), $4d^9nd$ ($n = 5, 6$), $4d^85s^2$, $4d^85s5d$, $5p^54d^{10}5p$, $5p^54d^{10}4f$ even configurations and the $4d^9np$ ($n = 5$–7), $4d^9nf$ ($n = 4$–6), $4d^85s5p$, $4d^85snf$ ($n = 4, 5$), $5p^54d^{10}5s$ and $5p^54d^{10}5d$ odd configurations, which are expected to take into account the most important configuration interaction effects relevant to this work.

The second, more extensive calculation (hereafter designated as HFR(B)) was that described in [17]. The following configurations were explicitly included in the physical model: $4d^{10}$ + $4d^9ns$ ($n = 5$–7) + $4d^9nd$ ($n = 5$–7) + $4d^9ng$ ($n = 5$–7) + $4d^85s^2$ + $4d^85p^2$ + $4d^85d^2$ + $4d^84f^2$ + $4d^86s^2$ + $4d^85s6s$ + $4d^85snd$ ($n = 5$–6) + $4d^86s6d$ + $4d^84f5p$ and $4d^9np$ ($n = 5$–7) + $4d^9nf$ ($n = 4$–7) + $4d^85snp$ ($n = 5$–6) + $4d^85snf$ ($n = 4$–6) + $4d^85pnd$ ($n = 5$–6) + $4d^84f5d$ for the even and odd parities, respectively. CPOL effects were also introduced in the model as a further refinement. More precisely, the core–valence correlation was considered within the framework of a CPOL potential and a correction to the dipole transition operator in a way described previously (see [22, 23]). The estimate of these contributions requires knowledge of the dipole polarizability of the ionic core, α_d, and of the cutoff radius, r_c. For the first parameter, we used the value computed by Fraga *et al* [29] for the $4s^24p^64d^8$ Ru-like Xe^{10+} ion, i.e. $\alpha_d = 0.61a_0^3$, while the cutoff radius, r_c, was chosen equal to $0.82a_0$ which corresponds to the mean HFR *r*-value of the outermost core orbital 4d.

In the two calculations, the HFR method has been combined with a least-squares optimization process in order to adjust the theoretical energy levels to the experimental values. With these sets of optimized parameters, we calculated the weighted oscillator strengths (log *gf*) and transition probabilities (*gA*) for the new transitions observed in the present investigation. The results are reported in table 3.

In the least-squares calculation for the even parity (HFR(A) calculation), we used the energy levels taken from the compilation by Saloman [13] that included the experimental values reported by Churilov [9] for the $4d^95s$,

Table 3. New 5s–5p, 5d–5f, 5p–5d, 5d–6p and 6s–6p classified lines of Xe IX, wavelengths, wavenumbers, weighted oscillator strengths and transition probabilities. For all the transitions, the core is $4d^9$.

					HFR(A)		HFR(B)	
Int.	λ_{vac} (Å)	$\sigma_{Obs.}$ (cm^{-1})	Δ	Classification	log *gf*	*gA* (s^{-1})	log *gf*	*gA* (s^{-1})
2	434.42	230 192	1	5d $^3S_1$–5f $^3P^\circ_2$	0.13	4.07E+10	0.07	3.54E+10
2	441.96	226 265	11	5p $^3F^\circ_3$–5d $^3G_3$	−1.40	1.37E+09	−1.36	1.48E+09
5	445.69	224 371	4	5d $^3D_3$–5f $^3G^\circ_4$	−2.31^b	1.65E+08^b	−2.16^b	2.34E+08^b
1	447.84	223 294	1	5d $^1P_1$–5f $^3F^\circ_2$	−0.31	5.90E+10	−0.39	1.21E+10
1	449.71	222 365	−8	5d $^1F_3$–5f $^3G^\circ_3$	−2.12^b	2.52E+08^b	−1.89^b	4.28E+08^b
2	453.21	220 648	6	5d $^3F_4$–5f $^3G^\circ_3$	−2.39	1.32E+08	−2.48	1.08E+08
2	454.32	220 111	4	5d $^1F_3$–5f $^3F^\circ_3$	−1.57	8.77E+08	−1.64	7.42E+08
3	454.97	219 795	3	5d $^3F_4$–5f $^3G^\circ_4$	−1.15	2.26E+09	−1.32	1.53E+09
3	457.68	218 493	−2	5d $^3D_3$–5f $^3P^\circ_2$	−1.87	4.25E+08	−2.15	2.27E+08
2	465.30	214 915	2	5d $^3P_2$–5f $^3D^\circ_2$	−1.20	2.05E+09	−1.37	1.40E+09
3	468.14	213 611	−3	5d $^1P_1$–5f $^3D^\circ_1$	−0.06	2.62E+10	−0.15	2.14E+10
4	470.66	212 468	3	5d $^3G_3$–5f $^3G^\circ_3$	−0.06	2.59E+10	−0.15	2.11E+10
2	475.13	210 469	2	5d $^3G_4$–5f $^3F^\circ_4$	−0.78	4.93E+09	−0.54	8.63E+09
2	485.38	206 024	−6	5d $^3F_2$–5f $^3G^\circ_3$	0.19	4.35E+10	0.09	3.49E+10
2	485.38	206 024	2	5d $^1F_3$–5f $^1F^\circ_3$	0.24	4.94E+10	0.13	3.82E+10
2	486.44	205 575	3	5d $^3P_0$–5f $^3D^\circ_1$	0.08	3.40E+10	0.01	2.90E+10
6bl	489.09	204 461	−1	5d $^1F_3$–5f $^1G^\circ_4$	0.73	1.49E+11	0.67	1.31E+11
6bl	489.14	204 440	0	5d $^3G_5$–5f $^3H^\circ_6$	1.09	3.45E+11	1.02	2.96E+11
1	492.24	203 153	−2	5d $^1G_4$–5f $^3G^\circ_4$	0.04	3.14E+11	−0.04	2.61E+10
5	493.09^a	202 803	−11	5p $^1P^\circ_1$–5d $^3D_1$	−0.50	8.63E+09	−0.66	6.01E+09
3	493.26	202 733	2	5d $^3F_4$–5f $^1G^\circ_4$	−3.77^b	4.64E+06^b	−1.34	1.27E+09
3	495.68	201 743	0	5d $^3F_3$–5f $^3F^\circ_3$	−0.12	2.04E+10	−0.19	1.75E+10
1	496.73	201 317	−2	5p $^1D^\circ_2$–5d $^3P_1$	−1.32	1.30E+09	−1.46	9.28E+08
2	497.13	201 155	−2	5d $^3F_4$–5f $^3F^\circ_3$	−0.46	9.33E+09	−0.51	8.38E+09
2	506.88	197 285	−2	5d $^3F_3$–5f $^3D^\circ_2$	−1.11	2.03E+09	−1.08	2.14E+09
3	509.91	196 113	−1	5d $^3G_3$–5f $^1F^\circ_3$	−1.24	1.47E+09	−1.09	2.08E+09
4	510.30	195 963	5	5d $^3S_1$–6p $^3P^\circ_0$	−2.06	2.23E+08	−1.92	3.05E+08
4	513.69^a	194 670	2	5p $^1F^\circ_3$–5d $^1D_2$	−0.67	5.37E+09	−0.75	4.50E+09
3	523.21	191 128	4	5d $^3D_2$–6p $^3D^\circ_2$	−3.42^b	9.25E+06^b	−2.69^b	5.08E+07^b
2	536.86^a	186 268	−2	5p $^3P^\circ_1$–5d $^3S_1$	−0.75	4.09E+09	−0.82	3.49E+09
5	543.24^a	184 081	−12	5p $^3D^\circ_2$–5d $^3G_3$	−0.65	5.07E+09	−0.76	3.89E+09
2	550.03	181 808	−2	5d $^1P_1$–6p $^1P^\circ_1$	−1.82	3.31E+08	−1.95	2.47E+08
5	582.90	171 556	−4	5d $^3G_5$–6p $^3F^\circ_4$	0.50	6.17E+10	0.51	6.39E+10
2	605.68	165 104	6	5d $^3D_2$–6p $^3F^\circ_3$	−0.78	3.06E+09	−0.82	2.77E+09
2	606.14	164 978	5	5d $^3D_1$–6p $^1P^\circ_1$	−0.82	2.76E+09	−1.05	1.62E+09
2	608.20	164 420	0	5d $^3P_0$–6p $^3P^\circ_1$	−0.68	3.81E+09	−0.71	3.48E+09
5	613.53	162 991	1	5d $^3D_1$–6p $^3F^\circ_2$	−1.43	6.62E+08	−1.48	5.98E+08
4	614.88	162 633	1	5d $^3D_3$–6p $^3F^\circ_3$	−0.21	1.09E+10	−0.23	1.05E+10
2	617.91	161 836	−3	5d $^1D_2$–6p $^1P^\circ_1$	−0.39	7.07E+09	−0.34	7.99E+09
3	623.03	160 506	0	5d $^1S_0$–5f $^3D^\circ_1$	−2.24	9.92E+07	−2.94^b	1.99E+07^b
3	631.27	158 411	1	5d $^3P_2$–6p $^3P^\circ_2$	−1.70	3.29E+08	−2.92^b	1.97E+07^b
1	640.81	156 052	1	5d $^1G_4$–6p $^3D^\circ_3$	−1.81	2.53E+08	−2.80^b	2.66E+07^b
1	696.09	143 659	4	5d $^1D_2$–6p $^3P^\circ_2$	−3.17^b	9.20E+06^b	−2.86^b	1.91E+07^b
3	707.09	141 424	0	5d $^3F_3$–6p $^3F^\circ_3$	−2.49^b	4.26E+07^b	−2.44^b	4.86E+07^b
2	715.92	139 680	−6	5s $^3D_3$–5p $^3F^\circ_2$	−2.35	5.73E+07	−2.42	4.90E+07

$4d^95d$ configurations, and by Raineri *et al* for the $4d^96s$ configuration [14]. The average energies (E_{av}) for the observed energy levels, the spin–orbit integrals (ζ_{nl}) and the monoconfigurational Slater integrals (F^k, G^k) were adjusted. To reduce the standard deviation, all the configuration–interaction integrals were scaled down at 85% of their HF values. The standard deviation of the fit was 212 cm^{-1}.

For the odd parity, in the least-squares calculation, we considered the energy level values reported in [13] and our new values for the $4d^96p$, $4d^94f$ and $4d^95f$ configurations. All the energy parameters were adjusted except the $G^3(4d, 6p)$ integral of the $4d^96p$ configuration that was fixed at 85% of its Hartree–Fock value, and the ζ_{4f} and $G^5(4d, 4f)$ integrals of the $4d^94f$ configuration that were fixed at the values calculated along the isoelectronic sequence according to [9, 11]. The spin–orbit parameter ζ_{5f} of the $4d^95f$ configuration was fixed at 95% of its Hartree–Fock value. All the interaction integrals were the HF values multiplied by 0.85. The standard deviation of the fit was 174 cm^{-1}.

The fits performed in the HFR(B) calculation were described previously [17] and will not be repeated here. The

Table 3. (Continued.)

Int.	λ_{vac} (Å)	$\sigma_{Obs.}$ (cm^{-1})	Δ	Classification	HFR(A) log *gf*	HFR(A) *gA* (s^{-1})	HFR(B) log *gf*	HFR(B) *gA* (s^{-1})
4	948.84	105 392	2	5s $^3D_1$–5p $^3P^\circ_2$	−2.56	2.05E+07	−2.58	1.96E+07
1	1276.45	78 342	0	6s $^1D_2$–6p $^3D^\circ_2$	−2.63[b]	9.52E+06[b]	−2.80[b]	6.88E+06[b]
1	1473.25	67 877	0	6s $^1D_2$–6p $^3F^\circ_2$	−1.65	6.96E+07	−0.99	3.29E+08
2	1570.42	63 677	−2	6s $^3D_3$–6p $^3D^\circ_3$	0.34	5.96E+09	0.36	6.68E+09
2	1613.71	61 969	−1	6s $^3D_2$–6p $^3D^\circ_2$	0.16	3.72E+09	0.18	4.18E+09
1	1712.21	58 404	0	6s $^3D_1$–6p $^3P^\circ_0$	−0.31	1.10E+09	−0.36	9.78E+08
2	1894.25	52 791	−3	6s $^3D_3$–6p $^3P^\circ_2$	0.31	3.73E+09	0.29	3.59E+09
3	1910.76	52 335	0	6s $^3D_1$–6p $^3F^\circ_2$	0.11	2.37E+09	0.10	2.41E+09

'bl' corresponds to a blended line.
[a] Previously classified by Garnir *et al* [17].
[b] Lines with the cancellation factor below 0.01 [19].
$\Delta = \sigma_{Obs.} - \sigma_{Calc.}$ (in cm^{-1}).

standard deviations were found to be equal to 207 cm^{-1} (even parity) and 164 cm^{-1} (odd parity), respectively.

The two sets of f values and transition probabilities are compared in table 4 while the parameter values used in this work (HFR(A) calculation) for both parities are presented in table 5. It is seen that the two sets of results agree generally well (within a few per cent for many transitions) if we consider the fact that the CPOL effects were included only in the HFR(B) calculation. For a few cases, larger discrepancies are observed but all of them can be explained by cancellation effects appearing in the calculation of the line strengths.

The lifetime values for the 6p and 5f levels, calculated with the HFR(A) and HFR(B) models, are compared in table 1. They agree quite well, the HFR(B) results appearing generally somewhat smaller than the HFR(A) lifetimes for the $4d^96p$ levels and somewhat larger than the HFR(A) values for the $4d^95f$ levels. This is mostly related to the inclusion of the CPOL effects in calculation B. The HFR(B) results are expected to be more accurate than the HFR(A) values because they include more configuration interaction effects, in a direct way, via the adopted set of configurations and, in an indirect way, via the CPOL contributions.

In order to further assess the reliability of the HFR calculations, as there are no experimental lifetime values available, we did additional calculations using the fully relativistic MCDF approach. We used the general purpose relativistic atomic structure package (GRASP) [20]. The computations were done with the extended average level (EAL) option, optimizing a weighted trace of the Hamiltonian using level weights proportional to $2J + 1$. The nuclear effects were estimated by considering a uniform charge distribution in the nucleus with the xenon atomic weight equal to 131.29. The following configurations were considered: $4d^{10}$, $4d^95s$, $4d^96s$, $4d^95d$, $4d^85s^2$, $4d^85p^2$, $4d^85d^2$, $4d^85s5d$ for the even parity and $4d^95p$, $4d^96p$, $4d^94f$, $4d^95f$, $4d^85s5p$, $4d^84f5s$ for the odd parity. This corresponds to 874 relativistic configuration state functions. This model is similar to that adopted in the work of Garnir *et al* [17], except that $4d^85p5d$, for computational reasons, was not included in the present calculation.

The lifetime values, calculated with the GRASP program, are presented in the last column of table 1 (Babushkin gauge).

Table 4. New 4d–4f classified lines of Xe IX. For all the transitions, the core is $4d^9$.

Int.	λ_{vac} (Å)	$\sigma_{Obs.}$ (cm^{-1})	Δ	Classification
3bl	691.63	144 586	0	4f $^3P^\circ_0$–5d $^3D_1$
3	849.71	117 687	0	4f $^3P^\circ_0$–5d $^3S_1$
2	883.65	113 167	−4	4f $^3D^\circ_3$–5d $^3G_3$
1	905.39	110 449	2	4f $^3F^\circ_3$–5d $^3F_2$
1	932.21	107 272	0	4f $^1G^\circ_4$–5d $^3F_3$
4	948.84	105 392	4	4f $^3D^\circ_2$–5d $^3P_1$
2	961.49	104 005	4	4f $^3D^\circ_3$–5d $^3P_2$
3	1001.55	99 845	−3	4f $^3H^\circ_4$–5d $^3G_5$
1	1024.26	97 631	3	4f $^3H^\circ_4$–5d $^3G_4$
3	1024.62	97 597	−1	4f $^3D^\circ_2$–5d $^3P_2$
1bl	1032.44	96 858	−2	4f $^3D^\circ_2$–5d $^1F_3$
1	1043.40	95 841	6	4f $^3F^\circ_3$–5d $^3F_4$
2	1053.07	94 960	−4	4f $^3F^\circ_4$–5d $^3G_5$
2	1053.07	94 960	0	4f $^3G^\circ_3$–5d $^1G_4$
3	1057.75	94 540	0	4f $^3D^\circ_1$–5d $^1P_1$
1bl	1062.65	94 104	0	4f $^3F^\circ_3$–5d $^1F_3$
1	1077.20	92 747	3	4f $^3F^\circ_4$–5d $^3G_4$
2	1083.16	92 322	0	4f $^3G^\circ_4$–5d $^1G_4$
2	1161.57	86 090	3	4f $^1F^\circ_3$–5d $^1D_2$
1	1276.45	78 342	2	4f $^3G^\circ_4$–5d $^1F_3$
2bl	1279.82	78 136	2	4f $^3G^\circ_3$–5d $^3D_3$
1	1321.71	75 660	−8	4f $^3G^\circ_3$–5d $^3D_2$
2	1416.60	70 592	−2	4f $^1F^\circ_3$–5d $^1F_3$
2	1531.83	65 281	−3	4f $^1F^\circ_3$–5d $^3D_2$

'bl' corresponds to a blended line.
$\Delta = \sigma_{Obs.} - \sigma_{Calc.}$ (in cm^{-1}).

The differences between the Babushkin and Coulomb gauges (velocity and length forms of the electric transition operators in the non-relativistic limit) are less than 10% for the $4d^95f$ configuration and do not exceed 20% on average for the $4d^96p$ configuration. As appears from the last three columns of table 1, the three sets of results, i.e. HFR(A), HFR(B) and GRASP, generally agree well, two notable exceptions being the 6p $^3P^\circ_1$ and 6p $^1P^\circ_1$ levels for which the two HFR calculations are in excellent agreement but consistently smaller than the MCDF results. The explanation probably must be found in the fact that these two levels are strongly perturbed as it

Table 5. Parameter values (in cm^{-1}) of the $4d^{10}$, $4d^9 5s$, $4d^9 6s$, $4d^9 5d$, $4d^9 5p$, $4d^9 6p$, $4d^9 4f$ and $4d^9 5f$ configurations of Xe IX. Configuration–interaction parameters are not quoted in this table. The standard deviations of the fits are 212 cm^{-1} (even parity) and 174 cm^{-1} (odd parity), respectively.

Configuration	Parameter	HFR value	Fitted value	Fitted/ HFR
$4d^{10}$	E_{av}	0	1 968 ± 213	–
$4d^9 5s$	E_{av}	465 886	463 562 ± 109	0.995
	ζ_{4d}	6 397	6 602 ± 91	1.032
	G^2(4d,5s)	18 818	16 421 ± 1037	0.873
$4d^9 6s$	E_{av}	908 208	909 102 ± 108	1.001
	ζ_{4d}	6 447	6661 ± 86	1.033
	G^2(4d,5s)	5 128	4 730 ± 1059	0.922
$4d^9 5d$	E_{av}	799 545	799 728 ± 54	1.000
	ζ_{4d}	6 439	6 630 ± 46	1.029
	ζ_{5d}	1 181	1 372 ± 67	1.161
	F^2(4d,5d)	32 601	26 937 ± 525	0.826
	F^4(4d,5d)	15 409	14 943 ± 688	0.970
	G^0(4d,5d)	7 693	6 083 ± 34	0.791
	G^2(4d,5d)	9 743	9 374 ± 584	0.962
	G^4(4d,5d)	8 196	4 421 ± 1213	0.539
$4d^9 5p$	E_{av}	602 574	603 356 ± 53	1.001
	ζ_{4d}	6 411	6 623 ± 51	1.033
	ζ_{5p}	12 984	14 176 ± 99	1.092
	F^2(4d,5p)	45 049	38 146 ± 522	0.847
	G^1(4d,5p)	13 486	12 183 ± 176	0.903
	G^3(4d,5p)	13 294	13 840 ± 968	1.041
$4d^9 6p$	E_{av}	966 820	968 048 ± 63	1.001
	ζ_{4d}	6 449	6 456 ± 49	1.001
	ζ_{6p}	5 472	5 517 ± 83	1.008
	F^2(4d,6p)	17 259	13 346 ± 562	0.773
	G^1(4d,6p)	4 167	3 694 ± 242	0.886
	G^3(4d,6p)	4 455	3 787 (Fixed)	0.850
$4d^9 4f$	E_{av}	701 710	701 052 ± 50	0.999
	ζ_{4d}	6 294	5 923 ± 83	0.941
	ζ_{4f}	362	228 (Fixed)	0.630
	F^2(4d,4f)	94 874	90 379 ± 469	0.953
	F^4(4d,4f)	60 385	46 380 ± 792	0.768
	G^1(4d,4f)	113 246	94 400 ± 124	0.833
	G^3(4d,4f)	70 166	58 342 ± 703	0.831
	G^5(4d,4f)	49 368	45 790 (Fixed)	0.927
$4d^9 5f$	E_{av}	1005 134	1004 770 ± 47	0.999
	ζ_{4d}	6 429	6 519 ± 37	1.014
	ζ_{5f}	127	121 (Fixed)	0.950
	F^2(4d,5f)	26 275	22 352 ± 677	0.850
	F^4(4d,5f)	13 711	14 804 ± 1383	1.080
	G^1(4d,5f)	18 175	11 359 ± 176	0.625
	G^3(4d,5f)	13 029	12 276 ± 859	0.942
	G^5(4d,5f)	9 683	6 248 ± 1258	0.645

appears from column 3 of table 1. In the $4d^9 6p$ configuration, we observe that the HFR(B) results appear, in many cases, slightly but significantly lower than the HFR(A) results. A similar situation is encountered in the $4d^9 5f$ configuration but, in this case, the HFR(B) lifetimes are systematically larger than the HFR(A) data. These trends are obviously due to the inclusion of the CPOL effects in the HFR(B) calculation.

The $4d^9 4f$ configuration deserves special attention. Most of the levels within this configuration are metastable and, consequently, have very long lifetimes (reaching typically 1 μs or so). These lifetime values are extremely sensitive to small configuration interaction effects and, consequently, to the choice of the sets of configurations adopted in the models. Most of these lifetimes are consequently 'unstable' in the sense that a modification of the selected configuration sets can, in some cases, induce very large modifications in the lifetime values. This is illustrated by the discrepancies observed between the HFR(A) and HFR(B) values for these levels and also by the considerable discrepancies observed between the two gauges when using the GRASP code. In addition, accurate calculations of lifetime values in the $4d^9 4f$ configuration would require to consider in a detailed way the contributions of the M1 and E2 forbidden transitions. For many of the $4d^9 4f$ levels, these contributions are negligible (smaller than 0.1%) but, for some, they are not. For the $^3H^\circ_4$ level, the E2 channel does contribute to the total decay by about 2% (the M1 contribution being negligible). For the $^1G^\circ_4$ level, the M1 and the E2 contributions reach about 2% and 9% of the E1 channels. For the $^3H^\circ_6$, $^3H^\circ_5$, $^1H^\circ_5$ and $^3G^\circ_5$ levels, the role of the forbidden transitions becomes of course primordial because the lifetime values of these levels are dictated only by these forbidden lines, the E1 decays being forbidden. As there are no experimental lifetimes available to test unambiguously the accuracy of the different lifetime calculations in this $4d^9 4f$ configuration, we have preferred not to quote lifetime values in table 2. For the same reason, we do not report in table 4 the f and A values for the transitions involving the $4d^9 4f$ configuration.

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