Electric Dipole Transition Parameters for 5*s*−5*p* and 5*p*−5*d* Transitions in Doubly Ionized Xenon

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Using the general-purpose relativistic atomic structure package based on the fully relativistic multiconfiguration Dirac–Fock method, we have reported the electric dipole transition (E1) parameters such as wavelengths, weighted oscillator strengths, transition rates (or probabilities) and line strengths for $5s-5p$ and $5p-5d$ transitions in Xe^{2+}. In calculations, the Breit interaction and quantum electrodynamic effects have been included as perturbations. The calculated values for energy levels including valence and core-valence correlation have been compared with other available experimental and theoretical values in literature. Our transition results can provide useful data for, in particular, experimental works in future.

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1. Introduction

Between the noble gases, xenon has some peculiarities in spectroscopy and electron dynamics. As a mid-Z element, xenon is strongly affected by electron correlations and xenon has a rather large fine-structure splitting because of the strong spin–orbit interaction [1]. The doubly ionized xenon atom, Xe^{2+} (Te-like), has the $5s^2\ 5p^4$ ground-state configuration. The true ground level in each case is $5p^4\ {}^3P_2$, followed by ${}^3P_0$, ${}^3P_1$, ${}^1D_2$ and ${}^1S_0$ in the same configuration [2]. Investigation of ionized xenon spectra is important for many reasons. Xenon has always had an important role in the development of lasers and laser techniques and is also an important element for light sources and development of lamps because of its rich emission spectrum. Te-like xenon is interesting for astrophysics as well, for example it was identified in the planetary nebula NGC 7027. Furthermore, there is an interest in spectroscopic and atomic data of xenon ions [3]. In addition, various atomic parameters such as energy levels, oscillator strengths, transition probabilities and radiative lifetimes have many important astrophysical applications. For example, transition probabilities are needed for calculating the energy transport through the star in model atmospheres and for direct analysis of stellar chemical compositions [4].

Various atomic parameters for Xe^{2+} were reported. The radiative lifetime of the ${}^1S_0$ metastable state of Xe^{2+} was measured by Walch and Knight [5], Calamai and Johnson [6], and Bhushan et al. [7], and studied by Hansen and Persson [8], Garstang [9], and Schippers et al. [10] theoretically. Saloman [11] compiled the energy levels and observed spectral lines of the xenon atom, in all stages of ionization for which experimental data were available. Andersen et al. [12] presented experimental results about cross-sections for the photoionization of $4d$ electrons in Xe^{+} and Xe^{2+} ions. Persson and Wahlström [13] investigated spectrum of doubly ionized xenon and compared this data with results of the Hartree–Fock calculations. Dzuba and Flambaum [14] calculated energy levels and Landé g factors for neutral xenon and all its positive ions from X II to Xe VIII. Using relativistic Hartree–Fock method, Sobral et al. [15] and Almandos et al. [4] presented astrophysical and laser studies for several xenon ions. The results of calculations of the transition probabilities of forbidden lines for a number of atoms and ions of astrophysical or laboratory interest were obtained by Osterbrock [16]. Gallardo and co-workers [17] presented the structure of the $5^2 5p^3$ $({}^4S)$ nl level system of Xe III. Bolognesi et al. [18] measured the doubly charged states of Xe and their associated satellite states over the energy range 33–54.5 eV by threshold photoelectron–threshold photoelectron coincidence (TPEsCO) spectroscopy. Four-component implementation of the two-particle (2p) propagator as a powerful tool for calculating double-ionization spectra of systems containing heavy elements were reported by Pernpointner [19].

In this work, the calculations have been performed by the general-purpose relativistic atomic structure package, GRASP [20]. This code includes the Breit interactions (magnetic interaction between the electrons and retardation effects of the electron-electron interaction) for relativistic effects and quantum electrodynamical (QED) contributions (self-energy and vacuum polarization). In addition, we have here taken into account the configurations including electron excitations from the valence $5p$ to other high sub-shell (valence correlation) and electron excitation from $5s$ subshell to other high subshells (core-valence correlation). Therefore the configuration set of $5s^2\ 5p^4$, $5p^6$, $5s5p^4 5d$, $5s^2 5p^2 5d^2$, $5p^4 5d^2$, $5s5p^5$, $5s^2 5p^3 5d$, $5p^5 5d$, $5s^2 5p 5d^3$, $5s^2 5p^3 6s$, $5s^2 5p^3 6p$, and $5s^2 5p^3 6d$ have been considered in calculations. The

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core $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}$ is common for all configurations and fixed calculations through.

2. Calculation method

Radiative properties of atoms are described on electromagnetic transition between two states, characterized by the angular momentum and parity of the corresponding photon. Once initial and final state functions have been calculated, the radiative matrix element for radiative properties computation can be obtained from

$$O_{if} = \left\langle \psi(i) \left| \boldsymbol{O}_q^{\pi(k)} \right| \right\rangle , \tag{1}$$

where $\boldsymbol{O}_q^{\pi(k)}$ is a spherical operator of rank k and parity π, and $\pi(k)$ is $\pi = (-1)^k$, for an electric multipole transition or $\pi = (-1)^{k+1}$, for a magnetic multipole transition. The largest transition probability is for electric dipole (E1) radiation, dominated by the least factor $1/\alpha^2$ over other types of transitions (E2, M1, M2, etc.). The transition probabilities (or rates) for the emission from the upper level to the lower level is given by

$$A^{\pi k}\left(\gamma' J', \gamma J\right) = 2C_k \left(\alpha \left(E_{\gamma' J'} - E_{\gamma J}\right)\right)^{2k+1} \times \frac{S^{\pi k}(\gamma' J', \gamma J)}{g_{J'}}, \tag{2}$$

where $S^{\pi k}$ is line strength,

$$S^{\pi k}\left(\gamma' J', \gamma J\right) = \left|\langle \gamma J || \boldsymbol{O}^{\pi(k)} || \gamma' J' \rangle\right|^2 , \tag{3}$$

where $C_k = (2k+1)(k+1)/[k((2k+1)!!)^2]$, and $\boldsymbol{O}^{\pi(k)}$ is transition operator.

Most experiments yield the lifetime of the upper level. In this case the sum over multipole transitions to all lower lying levels has to be taken. The lifetime, $\tau_{\gamma' J'}$, of upper level $\gamma' J'$ is

$$\tau_{\gamma' J'} = \frac{1}{\sum\limits_{\pi k, \gamma J} A^{\pi k}(\gamma' J', \gamma J)}. \tag{4}$$

The oscillator strength is a dimensionless quantity. It expresses radiation-induced electric dipole transitions between two states. For absorption, the oscillator strength is expressed by

$$f^{\pi k}(\gamma J, \gamma' J') = \frac{1}{\alpha} C_k \left(\alpha (E_{\gamma' J'} - E_{\gamma J})\right)^{2k-1} \times \frac{S^{\pi k}(\gamma J, \gamma' J')}{g_J}. \tag{5}$$

A similar expression can be written for the emission oscillator strength where $\gamma' J'$ and γJ are interchanged, making the emission oscillator strength negative.

3. Results and discussion

Atomic radiative transitions are important, especially in plasmas and astrophysics. In this paper, we have reported the electric dipole transition parameters including the excitation energies, wavelengths, oscillator strengths, transition probabilities, and line strengths for $5s$–$5p$ and $5p$–$5d$ transitions in doubly ionized xenon (Xe^{2+}) have been performed using the widely-used atomic structure package GRASP [20] based on the multiconfiguration Dirac–Fock method. In our calculations, we have used the option of extended average level (EAL) in GRASP code and selected the configuration set of $5s^2\,5p^4$, $5p^6$, $5s5p^45d$, $5s^25p^25d^2$, $5p^45d^2$, $5s5p^5$, $5s^25p^35d$, $5p^55d$, $5s^25p5d^3$, $5s^25p^36s$, $5s^25p^36p$ and $5s^25p^36d$. We have obtained 414 energy levels and 17205 possible electric dipole transitions (E1) for all levels obtained from above configurations. But we have here presented 39 low-lying fine structure levels and 75 E1 transition parameters for $5s$–$5p$ and $5p$–$5d$ transitions. Table I displays the energy levels of $5s^2\,5p^4$, $5s5p^5$ and $5s^25p^35d$. In the table, the contributions (from the Breit interaction and QED) have been also given in columns separately. We have compared our results including the Breit interaction and leading QED contributions (self-energy and vacuum polarization), and core-valence correlation with other works [14, 18, 19, 21] in literature. Results obtained are in agreement with others. In the last column of the table, we have given $\left(\frac{E_{tw}-E_{ow}}{E_{ow}}\right) \times 100\%$, the differences in per cent for the accuracy of the computed values, where E_{tw} and E_{ow} the energy values from this work and other works, respectively. When the differences between our results and other results in Ref. [21] is investigated, the differences are in the range of 0.004–18.79. In general, the energies for some levels of $5s^25p^35d$ are somewhat poor.

TABLE I

Energies, E [cm^{-1}], for the levels of $5s^2\,5p^4$, $5s5p^5$, and $5s^25p^35d$ configurations in Xe^{2+}. E^0: MCDF energies, E^1: Breit contributions, E^2: QED contributions, E^T: MCDF + Breit + QED.

Levels	E^0	E^1	E^2	E^T	Others	Diff. [%]
$5s^25p^4\ ^3P_2$	0.0000	0.00000	0.0000	0.00000	0.000	0.000
$5s^25p^4\ ^3P_0$	8061.30	–77.04	2.25	7986.68	8130.08^a, 7951.57^b, 8492.57^c, 8312.60^d	1.76
$5s^25p^4\ ^3P_1$	9112.59	–160.22	5.81	8957.86	9794.36^a, 9749.06^b, 9626.16^c, 9637.13^d	8.53
$5s^25p^4\ ^1D_2$	18914.32	–153.63	5.14	18766.18	17098.73^a, 17160.72^b, 17343.98^c, 19085.51^d	9.75
$5s^25p^4\ ^1S_0$	36363.65	–267.76	5.10	36101.38	36102.94^a, 35959.82^b, 37839.62^c, 37279.96^d	0.004
$5s5p^5\ ^3P_2^0$	98776.75	–129.49	–62.77	98584.71	98262.47^a, 98307.08^b, 98846.99^d	0.32
$5s5p^5\ ^3P_1^0$	104103.40	–201.92	–53.88	103847.72	103568.20^a, 103500.95^b, 104333.85^d	0.26
$5s5p^5\ ^3P_0^0$	108103.33	–283.12	–40.27	107779.60	108333.76^a, 109040.49^b, 108560.93^d	0.51
$5s^25p^3(^4S^0)5d\ ^5D_3^0$	112063.75	–314.95	2.13	111757.58	111605.41^a, 111693.93^b, 111365.82^d	0.13

TABLE I (cont.)

Levels	E^0	E^1	E^2	E^T	Others	Diff. [%]
$5s^25p^3(^4S^0)5d\ ^5D_2^0$	112447.83	–317.14	1.37	112132.88	111856.38^a, 111065.14^d	0.24
$5s^25p^3(^4S^0)5d\ ^5D_4^0$	112458.80	–336.89	2.28	112131.79	112271.78^a, 112274.44^b, 111365.82^d	0.12
$5s^25p^3(^4S^0)5d\ ^5D_1^0$	113095.28	–331.41	–2.49	112760.58	112448.90^a, 111505.19^d	0.27
$5s^25p^3(^4S^0)5d\ ^5D_0^0$	113698.83	–333.60	–14.27	113354.26	112693.95^a, 112661.82^b, 112141.66^d	0.58
$5s^25p^3(^4S^0)5d\ ^3D_2^0$	120645.21	–262.27	–0.82	120389.52	117240.08^a, 117210.43^b, 118574.46^d	2.61
$5s^25p^3(^2D^0)5d\ ^1P_1^0$	122664.37	–312.75	–22.72	122338.45	119026.03^a, 119001.34^d	2.78
$5s^25p^3(^4S^0)5d\ ^3D_3^0$	124448.70	–361.04	3.23	124092.06	121229.58^a, 121218.04^b, 122481.11^d	2.36
$5s^25p^3(^4S^0)5d\ ^3D_1^0$	125562.54	–365.43	0.60	125198.21	121922.75^a, 121710.76^b, 123250.37^d	2.68
$5s^25p^3(^2D^0)5d\ ^3F_2^0$	128930.37	–357.74	3.70	128580.31	124691.33^a, 124581.48^b, 127327.11^d	3.02
$5s^25p^3(^2D^0)5d\ ^3F_3^0$	130554.49	–375.30	4.18	130189.06	126119.77^a, 125952.10^b, 129044.50^d	3.12
$5s^25p^3(^2D^0)5d\ ^3F_4^0$	132343.21	–382.98	3.50	131971.20	130173.73^a, 129927.89^b, 133969.51^d	1.36
$5s^25p^3(^2D^0)5d\ ^3G_3^0$	134772.79	–303.97	1.78	134466.62	128349.15^a, 128186.36^b, 132921.52^d	4.76
$5s^25p^3(^2D^0)5d\ ^3G_4^0$	–	–	–	–	127782.14^a, 127621.21^b, 131306.19^d	–
$5s^25p^3(^2D^0)5d\ ^3G_5^0$	138258.05	–412.61	4.94	137850.92	132159.94^a, 132049.11^b, 136421.04^d	4.30
$5s^25p^3(^2D^0)5d\ ^1G_4^0$	139805.34	–378.59	4.55	139433.33	132711.78^a, 132621.94^b	5.06
$5s^25p^3(^2P^0)5d\ ^3P_0^0$	146170.11	–388.47	2.58	145822.24	140437.79^a, 140428.65^b	3.83
$5s^25p^3(^2P^0)5d\ ^3P_1^0$	146905.35	–367.62	0.79	146548.70	140730.93^a, 140662.39^b	4.13
$5s^25p^3(^2P^0)5d\ ^3F_3^0$	150219.41	–443.34	4.02	149788.15	145340.91^a	3.06
$5s^25p^3(^2P^0)5d\ ^3F_2^0$	151580.16	–430.17	4.96	151157.67	145300.13^a, 145283.43^b	4.03
$5s^25p^3(^2P^0)5d\ ^3P_2^0$	155486.81	–535.52	6.84	154968.85	150404.24^a	3.03
$5s^25p^3(^2P^0)5d\ ^3D_3^0$	159173.98	–388.47	1.77	158794.29	156393.68^a, 156283.50^b	1.51
$5s^25p^3(^2P^0)5d\ ^3D_1^0$	–	–	–	–	155400.90^a, 155291.47^b	–
$5s^25p^3(^2P^0)5d\ ^1F_3^0$	163354.97	–543.20	6.97	162822.74	162957.50^a, 162879.81^b	0.08
$5s^25p^3(^2P^0)5d\ ^3D_2^0$	148551.41	–389.57	4.50	148170.62	153893.20^a, 153791.36^b	3.86
$5s^25p^3(^2D^0)5d\ ^1D_2^0$	174229.94	–488.33	3.57	173748.19	161809.98^a, 161735.25^b	7.37
$5s^25p^3(^2P^0)5d\ ^1P_1^0$	189110.32	–465.29	–12.95	188635.16	175052.36^a	7.75
$5s^25p^3(^2D^0)5d\ ^3D_1^0$	–	–	–	–	133234.01^a, 133097.10^b	–
$5s^25p^3(^2D^0)5d\ ^3D_2^0$	–	–	–	–	142064.27^a, 142090.07^b	–
$5s^25p^3(^2D^0)5d\ ^3D_3^0$	152323.08	–414.81	4.70	151912.66	143156.24^a, 138218.54^b	6.11
$5s^25p^3(^2D^0)5d\ ^3S_1^0$	160580.81	–430.17	7.23	160157.2	147797.41^a, 147710.82^b	12.38
$5s^25p^3(^2D^0)5d\ ^3P_2^0$	171745.49	–417.00	–7.36	171320.80	148370.13^a, 148356.07^b	15.40
$5s^25p^3(^2D^0)5d\ ^3P_1^0$	174089.48	–369.81	–18.55	173701.00	154639.37^a, 154436.62^b	12.32
$5s^25p^3(^2D^0)5d\ ^3P_0^0$	178716.00	–454.31	–16.13	178245.22	160733.77^a	10.89
$5s^25p^3(^2D^0)5d\ ^1F_3^0$	176795.60	–500.40	5.28	176300.68	148412.84^a	18.79

^{a} Refs. [21; 13], ^{b} Ref. [18], ^{c} Ref. [19], ^{d} Ref. [14]

TABLE II

Wavelengths, λ [Å], transition probabilities, A_{IJ}, [s^{-1}], oscillator strengths, F_{JI}, line strengths, S_{IJ}, and the ratio of velocity and length gauge for the electric dipole (E1) transitions between the $5s$–$5p$ and $5p$–$5d$ levels in Xe^{2+}. The number in brackets represents the power of 10.

Transitions			λ		A_{IJ}	F_{JI}	S_{IJ}	Ratio
			NIST [21]	This work	This work	This work	This work	This work
$5s^2\ 5p^4$	$^3P_2 - 5s5p^5$	$^1P_1^0$	611.511	–	–	–	–	–
$5s^2\ 5p^4$	$^3P_1 - 5s5p^5$	$^1P_1^0$	650.479	–	–	–	–	–
$5s^2\ 5p^4$	$^1D_2 - 5s5p^5$	$^1P_1^0$	682.926	–	–	–	–	–
$5s^2\ 5p^4$	$^1S_0 - 5s5p^5$	$^1P_1^0$	784.785	–	–	–	–	–
$5s^2\ 5p^4$	$^3P_2 - 5s5p^5$	$^3P_1^0$	965.548	962.94	8.9191(6)	7.4392(–4)	1.1792(–2)	0.26
$5s^2\ 5p^4$	$^3P_1 - 5s5p^5$	$^3P_0^0$	1014.82	1011.9	1.0896(7)	5.5759(–4)	5.5726(–3)	0.22
$5s^2\ 5p^4$	$^3P_2 - 5s5p^5$	$^3P_2^0$	1017.68	1014.4	1.5854(7)	2.4455(–3)	4.0832(–2)	0.19
$5s^2\ 5p^4$	$^3P_0 - 5s5p^5$	$^3P_1^0$	1047.79	1043.2	1.2294(7)	6.0171(–3)	2.0664(–2)	0.41
$5s^2\ 5p^4$	$^3P_1 - 5s5p^5$	$^3P_1^0$	1066.39	1053.9	7.9324(6)	1.3208(–3)	1.3747(–2)	0.19
$5s^2\ 5p^4$	$^3P_1 - 5s5p^5$	$^3P_2^0$	1130.35	1115.7	1.4250(7)	4.4325(–3)	4.8844(–2)	0.29
$5s^2\ 5p^4$	$^1D_2 - 5s5p^5$	$^3P_1^0$	1156.47	1175.3	9.7879(6)	1.2163(–3)	2.3531(–2)	0.14
$5s^2\ 5p^4$	$^1D_2 - 5s5p^5$	$^3P_2^0$	1232.07	1252.9	4.0778(6)	9.5957(–4)	1.9789(–2)	0.18

TABLE II (cont.)

Transitions			λ		A_{IJ}	F_{JI}	S_{IJ}	Ratio
			NIST [21]	This work	This work	This work	This work	This work
$5s^2\ 5p^4$	$^1S_0 - 5s5p^5$	$^3P_1^0$	1482.24	1476.1	1.7497(6)	1.7146(–3)	8.3319(–3)	0.002
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^1P_1^0$	633.089	588.69	2.7918(9)	8.7028(–2)	8.4332(–1)	1.2
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2P^0)5d$	$^3D_3^0$	639.419	629.75	1.6514(10)	1.3746	1.4249	0.82
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3P_1^0$	646.667	575.70	8.1147(9)	2.4192(–1)	2.2925	0.92
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^1D_2^0$	657.831	606.83	8.6542(7)	7.9628(–3)	4.7724(–2)	0.73
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3P_0^0$	662.516	590.71	2.3647(10)	4.1235(–1)	2.4057	0.87
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2P^0)5d$	$^3P_2^0$	664.878	645.29	1.9869(7)	1.2404(–3)	1.3175(–2)	0.44
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^1F_3^0$	673.798	567.21	3.8690(7)	2.6126(–3)	2.4393(–2)	1.1
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3P_2^0$	673.991	583.70	6.7199(9)	3.4324(–1)	3.2978	0.89
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3S_1^0$	676.602	624.38	7.9010(9)	2.7707(–1)	2.8477	0.68
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^2P^0)5d$	$^3D_1^0$	679.022	–	–	–	–	–
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^2D^0)5d$	$^3P_1^0$	682.563	603.45	6.9749(9)	1.1423	2.2694	0.86
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^1F_3^0$	685.599	694.18	4.2727(6)	4.3214(–4)	4.9378(–3)	1.2
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^3D_1^0$	686.792	–	–	–	–	–
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2P^0)5d$	$^3F_3^0$	688.044	667.61	3.5445(8)	3.3157(–2)	3.6437(–1)	0.70
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2P^0)5d$	$^3F_2^0$	688.239	661.56	1.4373(8)	9.4307(–3)	1.0270(–1)	0.57
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3P_1^0$	690.400	607.01	7.0363(9)	3.8867(–1)	2.3301	0.84
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^1D_2^0$	691.036	645.24	1.7918(10)	1.1184	1.18781	0.75
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^3D_2^0$	693.971	718.33	6.9983(8)	9.0229(–2)	6.4012(–1)	0.70
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3D_3^0$	698.550	658.27	6.1234(9)	5.5692(–1)	6.0345	0.74
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3D_2^0$	703.906	–	–	–	–	–
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2P^0)5d$	$^3P_1^0$	710.575	682.37	1.0756(9)	4.5050(–2)	5.0601(–1)	0.56
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^3P_2^0$	711.190	684.88	5.1619(7)	6.0499(–3)	4.0922(–2)	0.68
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^2D^0)5d$	$^3S_1^0$	715.986	657.16	3.8926(9)	7.5606(–1)	1.6357	0.66
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3D_3^0$	717.911	714.15	1.2747(8)	1.3645(–2)	1.6039(–1)	0.85
$5s^2\ 5p^4$	$^1S_0 - 5s^25p^3(^2P^0)5d$	$^1P_1^0$	719.694	655.59	1.4056(10)	2.7170	5.8641	0.83
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3P_2^0$	721.630	615.91	8.0652(9)	7.6444(–1)	4.6500	0.86
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3D_1^0$	723.055	–	–	–	–	–
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3S_1^0$	724.623	661.38	3.7056(9)	2.4300(–1)	1.5873	0.60
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3P_1^0$	727.042	645.44	1.7985(7)	6.7395(–4)	7.1602(–3)	0.035
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3D_2^0$	731.023	772.78	2.6458(8)	2.3687(–2)	3.0131(–1)	0.40
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2P^0)5d$	$^1D_2^0$	733.314	–	–	–	–	–
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^3F_2^0$	737.977	703.24	1.2944(9)	1.5994(–1)	1.1109	0.73
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3P_2^0$	750.160	734.20	1.2669(8)	1.0239(–2)	1.2374(–1)	0.44
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^2P^0)5d$	$^3P_1^0$	754.144	721.70	3.8991(8)	9.1340(–2)	2.1702(–1)	0.72
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3D_2^0$	756.031	–	–	–	–	–
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^1F_3^0$	761.532	634.78	2.3166(10)	1.9593	2.04721	0.84
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3P_2^0$	761.790	655.50	1.5201(8)	9.7925(–3)	1.0566(–1)	0.46
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^3P_1^0$	763.729	726.80	9.7598(8)	7.7290(–2)	5.5479(–1)	0.72
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3S_1^0$	765.120	707.26	7.9105(6)	3.5593(–4)	4.1437(–3)	0.58
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^3P_0^0$	765.442	730.65	4.6976(8)	1.2532(–2)	9.0435(–2)	0.95
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3G_3^0$	779.124	743.68	2.7412(8)	3.1820(–2)	3.8952(–1)	0.79
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3F_3^0$	779.782	763.23	1.9549(8)	2.3902(–2)	3.0028(–1)	0.84
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3F_2^0$	780.027	755.34	2.3242(9)	1.9879(–1)	2.4716	0.63
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2P^0)5d$	$^1D_2^0$	790.056	–	–	–	–	–
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3F_3^0$	792.896	768.12	1.0792(8)	1.3364(–2)	1.6897(–1)	0.97
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3D_3^0$	793.282	751.06	2.7364(8)	3.2397(–2)	4.0052(–1)	0.66
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^2D^0)5d$	$^3D_1^0$	799.333	–	–	–	–	–
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3D_2^0$	800.228	–	–	–	–	–
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^3F_2^0$	801.978	777.73	6.1134(7)	5.5436(–3)	7.0968(–2)	0.90
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^3P_1^0$	808.860	782.59	5.1285(7)	2.8252(–3)	3.6394(–2)	0.67
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3D_1^0$	810.110	–	–	–	–	
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^4S^0)5d$	$^3D_1^0$	820.166	798.74	4.9984(6)	2.8684(–4)	3.7713(–3)	1.5

TABLE II (cont.)

Transitions			λ		A_{IJ}	F_{JI}	S_{IJ}	Ratio
			NIST [21]	This work	This work	This work	This work	This work
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^4S^0)5d$	$^3D_3^0$	824.878	805.86	7.0399(7)	9.5954(–3)	1.2728(–1)	1.1
$5s^2\ 5p^4$	$^1S_0 - 5s^25p^3(^2P^0)5d$	$^3D_1^0$	838.244	–	–	–	–	–
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2P^0)5d$	$^1D_2^0$	838.441	–	–	–	–	
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^2D^0)5d$	$^1P_1^0$	840.151	817.40	2.2912(7)	1.3770(–3)	1.8528(–2)	1.1
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^4S^0)5d$	$^3D_2^0$	852.947	830.64	8.0273(7)	8.3032(–3)	1.1353(–1)	1.0
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3D_1^0$	861.064	–	–	–	–	–
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^3F_2^0$	870.342	835.97	1.8768(7)	3.2772(–3)	2.7058(–2)	1.3
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^4S^0)5d$	$^3D_1^0$	878.789	853.17	5.4974(7)	1.7997(–2)	5.0549(–2)	1.3
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^4S^0)5d$	$^5D_1^0$	889.284	886.83	3.7448(7)	2.6492(–3)	3.8672(–2)	0.65
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^4S^0)5d$	$^3D_1^0$	891.835	860.30	6.7833(7)	7.5265(–3)	6.3949(–2)	1.0
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^4S^0)5d$	$^5D_2^0$	894.003	891.80	4.4321(7)	5.2844(–3)	7.7573(–2)	0.69
$5s^2\ 5p^4$	$^3P - 5s^25p^3(^4S^0)5d$	$^5D_3^0$	896.014	894.79	4.1784(7)	7.0216(–3)	1.0342(–1)	0.84
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3G_3^0$	898.870	864.30	5.3097(7)	8.3251(–3)	1.1844(–1)	0.92
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^2D^0)5d$	$^1P_1^0$	901.745	874.50	9.2487(6)	3.1811(–3)	9.1581(–3)	0.81
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^2D^0)5d$	$^1P_1^0$	915.487	881.99	2.2365(7)	2.6083(–3)	2.2720(–2)	0.79
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^3F_3^0$	917.258	897.49	1.3278(7)	2.2448(–3)	3.3163(–2)	0.89
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^4S^0)5d$	$^3D_2^0$	930.702	897.42	1.9411(7)	3.9061(–3)	3.4621(–2)	1.4
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^4S^0)5d$	$^3D_1^0$	953.983	939.58	8.3226(6)	6.6089(–4)	1.0221(–2)	0.071
$5s^2\ 5p^4$	$^3P_0 - 5s^25p^3(^4S^0)5d$	$^5D_1^0$	958.591	954.44	3.1982(6)	1.3103(–3)	4.1172(–3)	0.34
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^4S^0)5d$	$^3D_3^0$	960.325	949.44	3.2788(5)	6.2035(–5)	9.6950(–4)	2.1
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^4S^0)5d$	$^5D_0^0$	971.818	957.89	5.7156(7)	2.6208(–3)	2.4794(–2)	0.52
$5s^2\ 5p^4$	$^3P_1 - 5s^25p^3(^4S^0)5d$	$^5D_1^0$	974.133	963.37	2.0550(7)	2.8592(–3)	2.7204(–2)	0.66
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^2D^0)5d$	$^1P_1^0$	981.097	965.51	3.7787(7)	3.1686(–3)	5.0358(–2)	0.065
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^4S^0)5d$	$^5D_1^0$	1048.75	1063.9	6.8403(5)	7.9643(–5)	1.2196(–3)	0.28
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^4S^0)5d$	$^5D_2^0$	1055.32	1071.1	3.9734(5)	6.8335(–5)	1.2047(–3)	0.14
$5s^2\ 5p^4$	$^1D - 5s^25p^3(^4S^0)5d$	$^5D_3^0$	1058.13	1075.4	1.4130(5)	3.4296(–5)	6.0708(–4)	0.72
$5s^2\ 5p^4$	$^1S_0 - 5s^25p^3(^4S^0)5d$	$^5D_1^0$	1309.81	1304.5	3.5978(5)	2.7535(–4)	1.1825(–3)	0.018

TABLE III

The radiative lifetime of the $^1S_0$ level for Xe^{2+}.

Lifetime value [ms]	Works
4.46±0.08	[5]
4.50±0.3	[6]
4.60±0.3	[7]
4.90	[8]
4.40	[9]
4.10	[10]
5.02	present work

In Table II, the wavelengths, transition rates (probabilities), oscillator strengths, and line strengths for electric dipole transition (E1) for $5s^2\ 5p^4{-}5s5p^5$ and $5s^2\ 5p^4{-}5s^25p^35d$ transitions in Xe^{2+} have been given in the length gauge. The ratios between the transition rates in the velocity and length gauges have been also shown in the last column of the table. In the table we have only compared the wavelength values with those of NIST [21]. Other electric dipole transition parameters such as transition probabilities, oscillator strengths and line strengths are firstly presented here. Some values for wavelengths are somewhat poor. Of course our transition results need other theoretical and experimental results for comparing. But for this ion, there are no data for these transitions in literature. We have not obtained the electric dipole transition parameters for some transitions which are in NIST [21] since the oscillator strengths of these transitions are probably zero. In addition we have calculated the radiative lifetime for $^1S_0$ state for ground configuration according to (4) and given in Table III. The lifetime value obtained for this state is in good agreement with those of other works [5–10] when comparing.

4. Conclusion

A systematic GRASP study of the electric dipole transition parameters for $5s{-}5p$ and $5p{-}5d$ transitions in doubly ionized xenon (Xe^{2+}) has been presented. The calculations have been performed using the widely-used atomic structure package GRASP based on the multiconfiguration Dirac–Fock method. We have shown the effects of the Breit interaction and QED contributions on the levels and transitions. For energy values and wavelengths, our results are in good agreement with other results in generally. Of course our results need other theoretical, and in particular experimental, works for accuracy of results for the transitions here studied. For the transitions here reported for this ion, there are no data except wavelengths in literature. Therefore we hope that our results, in particular for transitions, will be useful for the experimental and theoretical studies in future.

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