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Electric dipole transitions between low-lying levels in doubly ionized krypton, xenon, and radon

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Abstract: Using the general-purpose relativistic atomic structure package (GRASP) based on a fully relativistic multiconfiguration Dirac–Fock (MCDF) method, the transition parameters, such as transition rates (probabilities), oscillator strengths, and line strengths for the electric dipole transitions between low-lying levels are evaluated for doubly ionized krypton, xenon, and radon. Breit interactions for relativistic effects and quantum electrodynamical (QED) contributions besides valence and valence–core correlation effects are taken into account in calculations. We compare the results obtained with the available data in the literature and discuss them, when possible.

Key words: energies, correlation effects, Breit interactions, QED contributions, E1 transitions.

Résumé : Utilisant l'ensemble logiciel relativiste à utilisation générale (GRASP), basé sur une méthode de Dirac–Fock multi-configurations (MCDF), nous évaluons des paramètres de transitions, comme les taux (probabilités) de transition, les forces d'oscillateur et les intensités de raie pour les transitions dipolaires électriques (E1) entre les niveaux les plus bas dans des atomes doublement ionisés de krypton, de xénon et de radon. Les calculs tiennent compte de l'interaction de Breit pour les effets relativistes et des contributions d'électrodynamique quantique (QED), en plus des corrélations cœur-valence. [Traduit par la Rédaction]

Mots-clés : énergies, effets de correlation, interaction de Breit, contributions EDQ, transitions E1.

1. Introduction

Radiative transition parameters, such as transition probabilities, oscillator strengths, and line strengths are fundamental characteristics of excited states of atoms and ions. These data play an important role in plasma and laser investigations and astrophysics. To interpret observed spectra, knowledge of accurate transition parameters is necessary [1].

There are few electric dipole transition data for Kr III and Xe III, and no data for Rn III in the literature. Krypton (Z = 36), xenon (Z = 54), and radon (Z = 86) atoms are among the noble gases. The doubly ionized krypton (Kr III), xenon (Xe III), and radon (Rn III) atoms are isoelectronic with neutral selenium, tellurium, and polonium, respectively. These ions have ns^2np^4 electron ground configuration (n = 4, 5, and 6 for Kr III, Xe III, and Rn III, respectively). The ground level for ions is np^4 $^3P_2$, and this level is followed by $^3P_1$, $^3P_0$, $^1D_2$, and $^1S_0$ in the same configuration.

Krypton has been detected in the spectra of the interstellar medium and is present in many light sources and lasers as the working gas. In addition, the singly and doubly ionized krypton spectral lines are very useful for plasma diagnostic purposes [2]. There are studies, in particular on radiative lifetimes for metastable states and transition parameters for krypton ions [2–16]. Raineri et al. also reported the weighted oscillator strengths and spectral lines belonging to some transitions and compared multiconfigurational Hartree-Fock relativistic approach [17]. Saloman compiled observed spectral lines of the krypton atom (Kr I – Kr XXXVI) [18].

In the development of lasers and laser techniques, xenon has always had an important role and is also an important element for light sources and development of lamps because of its rich emission spectrum, and Xe III (Te-like) is interesting for astrophysics as well, for example, it was identified in the planetary nebula NGC 7027 [19]. For Xe III, there are some studies including lifetimes and radiative transition parameters, in particular metastable states [14, 15, 20–28]. Saloman compiled the energy levels and observed spectral lines of the xenon atom, in all stages of ionization for which experimental data were available [29].

Radon is a radioactive noble gas element, which is obtained by radioactive disintegration of radium, while all other noble gases are present in the atmosphere. Biémont and Quinet presented a theoretical study for Rn III [30]. Pernpointner et al. reported double ionization spectra of the noble gas atoms Ne through Rn [31].

In this work, we report radiative transition parameters, such as transition rates (probabilities), oscillator strengths, and line strengths for the electric dipole transitions in doubly ionized krypton (Se-like), xenon (Te-like), and radon (Po-like), using the general-purpose relativistic atomic structure package (GRASP) [32]. This code includes 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). These contributions are important in investigations including electronic structure and spectroscopic properties of many electron systems. In addition, we have taken into account the configurations including the excitations from valence and core.

2. Computational details

The GRASP code [32] is based on a fully relativistic multiconfiguration Dirac–Fock (MCDF) model, and uses Thomas–Fermi and

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Table 1. Configurations considered for calculations.

Ion	Configurations
Kr III	$4s^24p^4$, $4s4p^5$, $4p^6$, $4s^24p^35s$, $4p^55s$, $4s^24p^36s$, $4s^24p^35p$
Xe III	$5s^25p^4$, $5s5p^5$, $5p^6$, $5s5p^45d$, $5s^25p^25d^2$, $5p^45d^2$, $5s^25p^35d$, $5p^55d$, $5s^25p^36s$, $5s^25p^36p$, $5s^25p^36d$, $5s^25p^34f$
Rn III	$6s^26p^4$, $6s6p^5$, $6p^6$, $6s^26p^37s$, $6s^26p^37p$, $6s^26p^36d$, $6p^46d^2$, $6p^56d$, $6s6p^37s^2$, $6s6p^38s^2$, $6s^26p^26d7s$, $6p^47s^2$, $6s^26p^27s^2$, $6p^57s$, $6s^26p^37d$, $6p^46d7s$

Table 2. Transition probabilities, A_{ij} (s^{-1}), the logarithm of the weighted oscillator strength, log(*gf*), and line strengths, S_{ij} (a.u.), for the electric dipole (E1) transitions between some low-lying levels of Kr III.

Lower level		Upper level		A_{ij} (s^{-1})	log(*gf*) This work	log(*gf*) [17]	S_{ij} (a.u.)	Ratio
$4s^24p^4$	$^3P_2$	$4s4p^5$	$^3P^\circ_2$	6.269(9)	0.403	−0.664	6.105	0.84
$4s^24p^4$	$^3P_2$	$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	1.949(7)	−2.106	−1.897	0.019	0.79
$4s^24p^4$	$^3P_2$	$4s4p^5$	$^3P^\circ_1$	4.384(9)	−0.219	—	2.367	0.84
$4s^24p^4$	$^3P_2$	$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	3.639(9)	−0.323	−0.115	1.814	0.72
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	7.981(7)	−2.074	−1.703	0.028	0.82
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	1.142(9)	−0.474	—	0.687	0.76
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	2.010(9)	−0.092	0.215	1.650	0.75
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	1.266(8)	−1.454	−0.765	0.070	0.74
$4s^24p^4$	$^3P_1$	$4s4p^5$	$^3P^\circ_2$	1.919(9)	−0.083	−1.081	2.060	0.84
$4s^24p^4$	$^3P_1$	$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	2.369(6)	−2.993	−2.682	0.002	0.81
$4s^24p^4$	$^3P_1$	$4s4p^5$	$^3P^\circ_1$	1.848(9)	−0.345	−1.340	1.097	0.85
$4s^24p^4$	$^3P_1$	$4s4p^5$	$^3P^\circ_0$	8.819(9)	−0.633	−1.231	1.669	0.85
$4s^24p^4$	$^3P_1$	$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	2.254(9)	−0.282	−0.481	1.232	0.73
$4s^24p^4$	$^3P_1$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	1.277(9)	−0.624	−0.841	0.503	0.76
$4s^24p^4$	$^3P_1$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	8.635(8)	−0.573	−1.076	0.565	0.75
$4s^24p^4$	$^3P_1$	$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	2.511(8)	−1.133	−1.105	0.151	0.78
$4s^24p^4$	$^3P_0$	$4s4p^5$	$^3P^\circ_1$	2.471(9)	−0.214	−1.217	1.492	0.86
$4s^24p^4$	$^3P_0$	$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	9.342(8)	−0.660	−0.886	0.519	0.74
$4s^24p^4$	$^3P_0$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	7.016(8)	−0.879	—	0.280	0.75
$4s^24p^4$	$^1D_2$	$4s4p^5$	$^3P^\circ_2$	9.979(7)	−1.276	−1.971	0.146	0.80
$4s^24p^4$	$^1D_2$	$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	5.971(4)	−2.743	−3.345	0.000	0.64
$4s^24p^4$	$^1D_2$	$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	9.731(6)	−3.260	−2.535	0.007	0.63
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	1.577(8)	−1.678	−1.562	0.081	0.77
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	1.107(8)	−1.389	−1.335	0.094	0.71
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	5.115(7)	−1.586	−1.731	0.059	0.79
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	4.605(9)	0.204	0.237	3.589	0.74
$4s^24p^4$	$^1S_0$	$4s4p^5$	$^3P^\circ_1$	4.469(7)	−1.769	–	0.052	0.56
$4s^24p^4$	$^1S_0$	$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	4.076(5)	−3.834	–	0.000	0.80
$4s^24p^4$	$^1S_0$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	2.971(7)	−2.088	−3.209	0.021	0.71

Note: The number in brackets represents the power of 10.

Coulomb potentials to calculate wavefunctions according to JJ and LS coupling. In the MCDF method [33] an atomic state can be expanded as a linear combination of configuration state functions (CSFs)

$$\Psi_a(PJM) = \sum_{r=1}^{n_c} C_r(\alpha)|\gamma_r(PJM)\rangle \tag{1}$$

where n_c is the number of CSFs included in the evaluation of atomic state functions and C_r is the mixing coefficient; and is optimized usually on the basis of the many-electron Dirac–Coulomb Hamiltonian. This method is basic and requires no knowledge of the internal coupling of the CSFs with a given parity *P* and angular momentum (*J*, *M*). The CSFs are the sum of products of single-electron Dirac spinors,

$$\phi(r,\theta,\varphi,\sigma) = \frac{1}{r}\begin{bmatrix} P(r)\chi_{\kappa m}(\theta,\varphi,\sigma) \\ iQ(r)\chi_{-\kappa m}(\theta,\varphi,\sigma)\end{bmatrix} \tag{2}$$

where κ is a quantum number; $\chi_{\kappa m}$ is the spinor spherical harmonic in the LSJ coupling scheme; and $P(r)$ and $Q(r)$ are large and small radial components of one-electron wavefunctions represented on a logarithmic grid. The energy functional is based on the Dirac–Coulomb Hamiltonian in form

$$H_{DC} = \sum_{j=1}^{N}\left[(C\boldsymbol{\alpha}_j\cdot\boldsymbol{p}_j) + (\beta_j - 1)c^2 + V(r_j)\right] + \sum_{j<k}^{N}\frac{1}{r_{jk}} \tag{3}$$

where $V(r_j)$ is the monopole part of the electron–nucleon interaction. Once initial and final state functions have been calculated, the radiative matrix element for radiative properties computation can be obtained from

$$O_{if} = \langle\psi(i)|\boldsymbol{O}_q^{\pi(k)}|\psi(f)\rangle \tag{4}$$

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

Table 3. Transition probabilities, A_{ij} (s^{-1}), oscillator strengths, F_{ji}, and line strengths, S_{ij} (a.u.), for the electric dipole (E1) transitions between some low-lying levels of Xe III.

Lower level		Upper level		A_{ij} (s^{-1})	F_{ji}	S_{ij} (a.u.)	Ratio
$5s^25p^4$	$^3P_2$	$5s5p^5$	$^3P^\circ_2$	8.124(6)	0.001	0.020	0.830
$5s^25p^4$	$^3P_2$	$5s5p^5$	$^3P^\circ_1$	3.855(6)	0.000	0.004	1.400
$5s^25p^4$	$^3P_2$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_3$	4.142(7)	0.007	0.100	0.870
$5s^25p^4$	$^3P_2$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_2$	4.082(7)	0.005	0.069	0.810
$5s^25p^4$	$^3P_2$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_1$	3.171(7)	0.002	0.032	0.870
$5s^25p^4$	$^3P_2$	$5s^25p^3(^4S^\circ)5d$	$^3D^\circ_2$	9.110(7)	0.009	0.126	0.880
$5s^25p^4$	$^3P_2$	$5s^25p^3(^4S^\circ)6s$	$^5S^\circ_2$	1.839(8)	0.018	0.242	0.640
$5s^25p^4$	$^3P_0$	$5s5p^5$	$^3P^\circ_1$	8.299(6)	0.004	0.013	0.920
$5s^25p^4$	$^3P_0$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_1$	2.212(6)	0.000	0.002	0.700
$5s^25p^4$	$^3P_1$	$5s5p^5$	$^3P^\circ_2$	1.040(7)	0.003	0.034	0.610
$5s^25p^4$	$^3P_1$	$5s5p^5$	$^3P^\circ_1$	4.380(6)	0.000	0.007	0.720
$5s^25p^4$	$^3P_1$	$5s5p^5$	$^3P^\circ_0$	4.928(6)	0.000	0.002	1.200
$5s^25p^4$	$^3P_1$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_2$	9.288(5)	0.000	0.002	1.400
$5s^25p^4$	$^3P_1$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_1$	1.858(7)	0.002	0.024	0.820
$5s^25p^4$	$^3P_1$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_0$	4.190(7)	0.001	0.017	0.910
$5s^25p^4$	$^3P_1$	$5s^25p^3(^4S^\circ)5d$	$^3D^\circ_2$	2.465(7)	0.005	0.043	0.960
$5s^25p^4$	$^3P_1$	$5s^25p^3(^4S^\circ)6s$	$^5S^\circ_2$	8.460(6)	0.001	0.014	0.620
$5s^25p^4$	$^1D_2$	$5s5p^5$	$^3P^\circ_2$	3.118(6)	0.000	0.014	0.440
$5s^25p^4$	$^1D_2$	$5s5p^5$	$^3P^\circ_1$	5.293(6)	0.000	0.012	0.620
$5s^25p^4$	$^1D_2$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_3$	1.379(5)	0.000	0.000	1.300
$5s^25p^4$	$^1D_2$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_2$	8.164(5)	0.000	0.002	0.630
$5s^25p^4$	$^1D_2$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_1$	5.223(5)	0.000	0.000	0.420
$5s^25p^4$	$^1D_2$	$5s^25p^3(^4S^\circ)5d$	$^3D^\circ_2$	1.142(5)	0.000	0.000	0.001
$5s^25p^4$	$^1D_2$	$5s^25p^3(^4S^\circ)6s$	$^5S^\circ_2$	7.737(3)	0.000	0.000	0.460
$5s^25p^4$	$^1S_0$	$5s5p^5$	$^3P^\circ_1$	1.185(6)	0.001	0.006	0.062
$5s^25p^4$	$^1S_0$	$5s^25p^3(^4S^\circ)5d$	$^5D^\circ_1$	2.314(5)	0.000	0.000	0.120

Note: The number in brackets represents the power of 10.

Table 4. Transition probabilities, A_{ij} (s^{-1}), oscillator strengths, F_{ji}, and line strengths, S_{ij} (a.u.), for the electric dipole (E1) transitions between some low-lying levels of Rn III.

Lower level		Upper level		A_{ij} (s^{-1})	F_{ji}	S_{ij} (a.u.)	Ratio
$6s^26p^4$	$^3P_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_2$	9.971(8)	0.164	2.817	0.88
$6s^26p^4$	$^3P_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_2$	3.643(7)	0.006	0.096	0.41
$6s^26p^4$	$^3P_2$	$6s^26p^3(^4S^\circ)7s$	$^3S^\circ_1$	1.680(9)	0.158	2.663	0.88
$6s^26p^4$	$^3P_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_3$	2.469(8)	0.053	0.879	0.66
$6s^26p^4$	$^3P_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_1$	2.203(8)	0.020	0.327	1.40
$6s^26p^4$	$^3P_2$	$6s^26p^3(^2P^\circ)6d$	$^3P^\circ_2$	5.327(8)	0.078	1.273	0.63
$6s^26p^4$	$^3P_2$	$6s^26p^3(^2D^\circ)6d$	$^3G^\circ_3$	4.060(9)	0.640	9.126	0.63
$6s^26p^4$	$^3P_2$	$6s^26p^3(^4S^\circ)6d$	$^3D^\circ_1$	1.290(9)	0.085	1.207	0.80
$6s^26p^4$	$^3P_0$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_1$	1.176(8)	0.067	0.248	0.85
$6s^26p^4$	$^3P_0$	$6s^26p^3(^4S^\circ)6d$	$^3D^\circ_1$	2.701(9)	1.091	3.403	0.60
$6s^26p^4$	$^3P_1$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_2$	1.271(6)	0.000	0.011	2.40
$6s^26p^4$	$^3P_1$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_2$	4.086(5)	0.000	0.003	0.67
$6s^26p^4$	$^3P_1$	$6s^26p^3(^4S^\circ)7s$	$^3S^\circ_1$	3.081(6)	0.001	0.015	1.80
$6s^26p^4$	$^3P_1$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_1$	2.723(7)	0.008	0.120	1.10
$6s^26p^4$	$^3P_1$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_0$	1.190(7)	0.001	0.017	0.51
$6s^26p^4$	$^3P_1$	$6s^26p^3(^2P^\circ)6d$	$^3P^\circ_2$	8.049(6)	0.004	0.056	0.26
$6s^26p^4$	$^1D_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_2$	2.092(5)	0.000	0.003	0.39
$6s^26p^4$	$^1D_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_3$	1.130(5)	0.000	0.002	2.00
$6s^26p^4$	$^1D_2$	$6s^26p^3(^4S^\circ)6d$	$^5D^\circ_1$	5.329(5)	0.000	0.003	0.58
$6s^26p^4$	$^1D_2$	$6s^26p^3(^2P^\circ)6d$	$^3P^\circ_2$	8.851(5)	0.000	0.009	0.03
$6s^26p^4$	$^1D_2$	$6s^26p^3(^2D^\circ)6d$	$^3G^\circ_3$	2.605(6)	0.000	0.020	0.76
$6s^26p^4$	$^1D_2$	$6s^26p^3(^4S^\circ)6d$	$^3D^\circ_1$	4.956(6)	0.000	0.016	2.10

Note: The number in brackets represents the power of 10.

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 for the emission from the upper level to the lower level is given by

$$A^{\pi k}(\gamma' J', \gamma J) = 2C_k[\alpha(E_{\gamma' J'} - E_{\gamma J})]^{2k+1}\frac{S^{\pi k}(\gamma' J', \gamma J)}{g_{J'}} \tag{5}$$

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

$$S^{\pi k}(\gamma' J', \gamma J) = |\langle \gamma J || \boldsymbol{O}^{\pi(k)} || \gamma' J' \rangle|^2 \tag{6}$$

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

The oscillator strength is a dimensionless parameter. It is associated with radiation-induced electric dipole transitions between two states,

Table 5. Transition probabilities, A_{ij} (s^{-1}), logarithm of the weighted oscillator strength, log(gf), and line strengths, S_{ij} (a.u.), for the electric dipole (E1) transitions for some high levels in Kr III and Xe III.

Lower level		Upper level		A_{ij} (s^{-1})		log(gf)			
				This work	Other works	This work	Other work	S_{ij} (a.u.)	Ratio
Kr III									
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^3P_2$	1.93(8)	0.75(8)[a] 1.16(8)[b] 0.85(8)[c] 1.22(8)[d]	0.288	0.289[a]	23.372	1.0
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3F_2$	2.11(8)	0.08(8)[a] 1.10(8)[b] 0.97(8)[c] 1.59(8)[d]	0.289	0.202[a]	22.504	0.90
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^5P_1$	2.31(8)	0.89(8)[a] 0.86(8)[b] 1.11(8)[c] 0.94(8)[d]	–0.118	0.099[a]	14.587	0.89
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^5P_2$	2.34(8)	2.80(8)[a] 1.59(8)[b] 3.33(8)[c] 0.98(8)[d]	0.323	0.313[a]	23.959	0.89
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	1.58(8)	1.13(8)[a] 1.34(8)[b] 0.86(8)[c] 1.68(8)[d]	0.204	0.157[a]	19.355	0.98
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^3F_4$	2.35(8)	0.88(8)[a] 0.92(8)[b] 0.92(8)[c] 1.60(8)[d]	0.590	0.549[a]	44.860	0.92
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^5P_3$	2.55(8)	1.00(8)[abcd]	0.487	0.490[a]	34.238	0.89
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^3P_2$	2.59(8)	0.80(8)[a] 1.32(8)[c] 1.02(8)[d]	0.121	0.186[a]	18.822	0.86
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^3P_1$	2.57(5)	—	–2.216	–1.839[a]	0.312	2.1
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^3P_1$	2.20(5)	—	–2.077	–1.528[a]	0.254	2.2
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^3P_2$	2.67(5)	—	–1.784	–1.497[a]	0.490	2.3
$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_0$	7.22(5)	—	–2.966	–2.009[a]	0.058	3.1
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^3P_0$	8.92(5)	—	–2.461	–1.588[a]	0.301	2.5
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_1$	2.35(7)	—	–0.849	–1.311[a]	3.665	1.5
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_2$	8.95(5)	—	–1.491	–0.723[a]	0.207	2.6
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	2.52(6)	—	–1.444	–2.491[a]	0.516	1.3
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1P_1$	9.02(7)	—	–0.387	–0.950[a]	9.243	1.2
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^5P_1$	9.46(5)	—	–2.035	–1.698[a]	0.141	1.2
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_3$	3.21(6)	—	–1.269	–0.393[a]	0.709	0.88
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^5P_2$	2.37(6)	—	–1.203	–1.089[a]	0.569	1.1
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1F_3$	1.72(8)	—	0.438	–0.095[a]	35.077	1.0
$4s^24p^3(^2P^\circ)5p$	$^3D_3$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	5.48(5)	—	–1.856	–2.166[a]	0.226	2.8
$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	3.08(6)	—	1.575	–1.335[a]	0.297	0.84
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3D_1$	1.47(6)	—	–2.371	–2.472[a]	0.077	0.80
$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	2.19(8)	—	–0.052	–0.767[a]	8.757	0.62
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_1$	5.17(7)	—	–0.667	–0.232[a]	4.634	0.99
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	1.27(7)	—	–1.341	–1.240[a]	0.328	0.70
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3D_1$	7.07(7)	—	–0.294	–0.261[a]	6.194	1.1
$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_0$	6.57(6)	—	–2.475	–1.471[a]	0.106	1.0
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^3F_2$	3.40(6)	—	–1.599	–1.338[a]	0.431	0.82
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	1.62(7)	—	–1.312	–1.728[a]	0.892	1.1
$4s^24p^3(^2P^\circ)5p$	$^3D_1$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	8.77(5)	—	–1.924	–1.905[a]	0.167	2.4
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^3P_1$	1.91(8)	—	0.072	0.064[a]	14.390	1.1
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	2.75(7)	—	–0.688	–1.755[a]	2.135	0.69
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^4S^\circ)5p$	$^3P_0$	2.00(8)	—	–0.878	–0.368[a]	4.758	1.1
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^3F_3$	1.30(8)	—	0.278	0.203[a]	23.240	0.99
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	1.94(7)	—	–0.807	–0.696[a]	2.785	0.94
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3D_1$	1.62(8)	—	–0.164	–0.489[a]	6.920	0.64
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3D_1$	1.64(8)	—	–0.173	–0.369[a]	6.663	0.64
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	9.60(7)	—	–0.688	–0.830[a]	3.165	0.58
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3F_2$	1.20(7)	—	–0.952	–0.502[a]	1.302	1.1

Table 5 (*continued*).

Lower level		Upper level		A_{ij} (s^{-1})		log(*gf*)			
				This work	Other works	This work	Other work	S_{ij} (a.u.)	Ratio
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3D_3$	3.37(8)	—	0.515	0.092[a]	32.800	0.69
$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^1D_2$	1.49(8)	—	−0.012	0.162[a]	9.442	0.75
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^3D_3$	6.78(7)	—	−0.039	0.084[a]	10.779	0.94
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3F_3$	7.61(7)	—	0.001	0.056[a]	11.673	0.91
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	3.32(8)	—	0.340	0.078[a]	21.370	0.65
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2D^\circ)5p$	$^1F_3$	2.47(6)	—	−1.499	−0.357[a]	0.365	1.2
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1P_1$	2.26(6)	—	−2.129	−2.103[a]	0.142	0.97
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	1.70(7)	—	−0.772	−0.782[a]	2.032	0.85
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	4.13(6)	—	−1.675	−0.435[a]	0.182	0.50
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^1P_1$	7.55(7)	—	−0.390	−0.258[a]	4.665	0.91
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	7.32(7)	—	−0.633	−0.716[a]	2.040	0.57
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	1.84(7)	—	−1.246	−0.244[a]	0.490	0.59
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_3$	1.62(8)	—	0.296	−0.111[a]	22.214	0.87
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_0$	4.16(8)	—	−0.784	−0.430[a]	4.567	0.63
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1F_3$	3.30(6)	—	−1.415	−0.810[a]	0.422	0.85
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^1D_2$	2.31(8)	—	0.123	−0.896[a]	12.114	0.62
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1D_2$	3.94(8)	—	0.385	0.287[a]	22.914	0.78
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	1.90(8)	—	0.036	0.216[a]	9.869	0.55
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^1D_2$	4.69(7)	—	−0.617	−1.652[a]	2.085	0.63
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^3P_1$	3.69(6)	—	−2.067	−1.500[a]	13.754	0.87
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^4S^\circ)5p$	$^3P_2$	9.00(6)	—	−1.246	−0.946[a]	0.542	0.87
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3P_2$	4.88(7)	—	−0.494	−0.670[a]	3.125	0.94
$4s^24p^3(^2D^\circ)5p$	$^3P_1$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_2$	4.35(7)	—	−0.243	−0.009[a]	3.412	1.3
$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	4.13(6)	—	−1.675	−1.068[a]	0.182	0.5
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	2.48(8)	—	−0.244	−0.333[a]	9.129	0.7
$4s^24p^3(^4S^\circ)5p$	$^3P_2$	$4s^24p^3(^4S^\circ)6s$	$^5S^\circ_2$	4.27(6)	—	−1.518	−1.895[a]	0.308	0.91
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_0$	3.67(8)	—	−0.811	−0.631[a]	4.427	0.75
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	9.91(7)	—	−0.424	−0.697[a]	3.599	0.83
$4s^24p^3(^2P^\circ)5p$	$^3P_2$	$4s^24p^3(^2P^\circ)6s$	$^3P^\circ_1$	1.13(5)	—	−3.530	−1.283[a]	0.005	5.5
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3D_1$	1.98(7)	—	−1.478	−0.688[a]	0.456	0.44
$4s^24p^3(^2D^\circ)5p$	$^3P_1$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	1.28(7)	—	−1.072	−1.014[a]	0.831	1.2
$4s^24p^3(^2D^\circ)5p$	$^3P_2$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	8.23(7)	—	−0.106	0.006[a]	7.761	1.2
$4s^24p^3(^2P^\circ)5p$	$^3P_2$	$4s^24p^3(^2P^\circ)6s$	$^1P^\circ_1$	1.54(8)	—	−0.396	−1.472[a]	5.432	1.1
$4s^24p^3(^2P^\circ)5p$	$^1D_2$	$4s^24p^3(^2P^\circ)6s$	$^3P^\circ_1$	3.49(7)	—	−1.042	−1.023[a]	1.545	1.3
$4s^24p^3(^4S^\circ)5p$	$^3P_2$	$4s^24p^3(^4S^\circ)6s$	$^3S^\circ_1$	2.24(8)	—	−0.299	−0.082[a]	7.945	1.4
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	3.97(4)	—	−3.977	−1.548[a]	0.001	0.019
$4s^24p^3(^4S^\circ)5p$	$^3P_1$	$4s^24p^3(^4S^\circ)6s$	$^3S^\circ_1$	1.45(8)	—	−0.275	−0.288[a]	4.988	1.3
$4s^24p^3(^2D^\circ)5s$	$^1D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	1.23(7)	—	−1.786	−0.844[a]	0.200	0.26
$4s^24p^3(^2D^\circ)5p$	$^3F_4$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	2.74(8)	—	0.212	0.396[a]	18.618	0.84
$4s^24p^3(^4S^\circ)5p$	$^5P_3$	$4s^24p^3(^4S^\circ)6s$	$^5S^\circ_2$	3.21(8)	—	0.089	0.212[a]	15.112	0.76
$4s^24p^3(^2D^\circ)5p$	$^1F_3$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	3.03(6)	—	−1.634	−0.762[a]	0.207	0.68
$4s^24p^3(^2D^\circ)5p$	$^1P_1$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_2$	8.93(3)	—	−4.314	−2.098[a]	0.000	14
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1D_2$	7.16(6)	—	−1.457	−1.527[a]	0.294	0.69
$4s^24p^3(^2P^\circ)5p$	$^3D_3$	$4s^24p^3(^2P^\circ)5d$	$^3P^\circ_2$	2.99(8)	—	0.060	0.221[a]	14.192	0.83
$4s^24p^3(^2D^\circ)5p$	$^3D_2$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_2$	1.66(8)	—	−0.078	−1.394[a]	7.121	0.82
$4s^24p^3(^2D^\circ)5p$	$^3F_3$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_2$	9.59(7)	—	−1.436	0.055[a]	4.469	0.84
$4s^24p^3(^2D^\circ)5p$	$^3D_3$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	6.78(7)	—	−0.300	−0.373[a]	4.375	0.82
$4s^24p^3(^2D^\circ)5p$	$^1F_3$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	2.78(8)	—	0.017	0.115[a]	12.672	9.6
$4s^24p^3(^4S^\circ)5p$	$^5P_2$	$4s^24p^3(^4S^\circ)6s$	$^5S^\circ_2$	2.25(8)	—	0.067	0.058[a]	10.085	0.76
$4s^24p^3(^2P^\circ)5p$	$^3P_1$	$4s^24p^3(^2P^\circ)6s$	$^3P^\circ_1$	9.75(6)	—	−0.921	−0.772[a]	0.409	0.96
$4s^24p^3(^4S^\circ)5p$	$^5P_1$	$4s^24p^3(^4S^\circ)6s$	$^5S^\circ_2$	1.37(8)	—	−0.156	−0.157[a]	5.996	0.76
$4s^24p^3(^2P^\circ)5p$	$^3P_0$	$4s^24p^3(^2P^\circ)6s$	$^1P^\circ_1$	7.57(6)	—	−1.615	−2.752[a]	0.213	0.80
$4s^24p^3(^2P^\circ)5p$	$^3P_1$	$4s^24p^3(^2P^\circ)5d$	$^3P^\circ_2$	1.92(7)	—	−0.921	−0.951[a]	1.140	1.1
$4s^24p^3(^2P^\circ)5p$	$^3P_1$	$4s^24p^3(^2P^\circ)6s$	$^1P^\circ_1$	1.14(8)	—	−0.389	−0.847[a]	3.792	1.0
$4s^24p^3(^2D^\circ)5p$	$^3F_2$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_2$	1.15(7)	—	−1.213	−2.105[a]	0.537	0.77
$4s^24p^3(^2D^\circ)5p$	$^3D_2$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	1.84(7)	—	−0.913	−0.652[a]	1.012	0.76
$4s^24p^3(^2D^\circ)5p$	$^3F_3$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	1.55(8)	—	0.034	−0.340[a]	9.180	0.79
$4s^24p^3(^2P^\circ)5p$	$^3D_2$	$4s^24p^3(^2P^\circ)5d$	$^3P^\circ_2$	1.77(7)	—	−0.035	−1.059[a]	0.763	0.84
$4s^24p^3(^2D^\circ)5p$	$^1P_1$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	8.56(7)	—	−0.379	−0.207[a]	3.513	0.87
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3F_2$	2.14(6)	—	−2.093	−2.138[a]	0.060	0.49
$4s^24p^3(^2P^\circ)5p$	$^3D_3$	$4s^24p^3(^2P^\circ)6s$	$^1P^\circ_1$	2.82(7)	—	−1.307	−1.017[a]	0.688	0.76
$4s^24p^3(^2D^\circ)5p$	$^3D_2$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	2.02(7)	—	−1.037	−1.627[a]	0.745	0.67
$4s^24p^3(^2D^\circ)5p$	$^3F_3$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	2.97(6)	—	−1.993	−2.039[a]	0.118	0.86

Table 5 (*continued*).

Lower level		Upper level		A_{ij} (s^{-1})		log(*gf*)			
Lower level		Upper level		This work	Other works	This work	Other work	S_{ij} (a.u.)	Ratio
$4s^24p^3(^4S^\circ)5p$	$^5P_2$	$4s^24p^3(^4S^\circ)6s$	$^3S^\circ_1$	6.07(6)	—	−1.996	−1.387[a]	0.137	1.3
$4s^24p^3(^4S^\circ)5p$	$^5P_1$	$4s^24p^3(^4S^\circ)6s$	$^3S^\circ_1$	1.50(6)	—	−2.388	−1.788[a]	0.033	1.3
$4s^24p^3(^2D^\circ)5p$	$^3F_2$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	2.61(6)	—	−1.737	−0.340[a]	0.156	0.78
$4s^24p^3(^2P^\circ)5p$	$^3D_1$	$4s^24p^3(^2P^\circ)6s$	$^3P^\circ_1$	9.97(7)	—	−0.503	−0.579[a]	2.735	0.89
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	7.77(5)	—	−2.512	−2.073[a]	0.023	0.66
$4s^24p^3(^2D^\circ)5p$	$^3F_2$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	2.96(6)	—	−1.848	−1.585[a]	0.118	0.77
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^1P_1$	1.42(5)	—	−3.500	−3.012[a]	0.002	0.20
$4s^24p^3(^2P^\circ)5p$	$^3D_1$	$4s^24p^3(^2P^\circ)6s$	$^1P^\circ_1$	9.58(5)	—	−2.5790	−2.576[a]	0.021	1.5
$4s^24p^3(^2D^\circ)5p$	$^3D_1$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_2$	5.60(7)	—	−0.5881	−0.584[a]	2.107	0.81
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3D_1$	1.55(6)	—	−2.6723	−2.118[a]	0.026	0.42
$4s^24p^3(^2D^\circ)5p$	$^3D_1$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	2.63(7)	—	−0.959	−0.992[a]	0.855	0.85
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2P^\circ)5p$	$^3D_3$	1.50(7)	—	−1.116	−1.372[a]	0.011	0.55
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	4.06(6)	—	−1.832	−2.122[a]	0.107	0.38
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	8.24(6)	—	−1.528	−2.584[a]	0.214	0.37
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	7.78(6)	—	−2.064	−4.560[a]	0.096	0.16
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	2.83(5)	—	−3.761	−2.157[a]	0.003	1.3
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3D_3$	1.74(7)	—	−1.076	−4.372[a]	0.592	0.35
$4s^24p^3(^2D^\circ)5p$	$^1D_2$	$4s^24p^3(^2P^\circ)5d$	$^3P^\circ_2$	3.10(6)	—	−1.937	−1.593[a]	0.085	0.29
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_2$	6.93(7)	—	−0.683	−0.872[a]	1.363	0.55
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_0$	6.93(7)	—	−1.868	−1.686[a]	0.265	0.57
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	5.19(7)	—	−1.039	−1.190[a]	0.596	0.58
$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_3$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	1.871(7)	—	−1.373	−2.307[a]	0.401	0.28
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3F_3$	3.20(4)	—	−3.900	−2.812[a]	0.000	0.42
$4s^24p^3(^2D^\circ)5p$	$^3P_0$	$4s^24p^3(^2P^\circ)6s$	$^1P^\circ_1$	1.30(6)	—	−2.639	−4.254[a]	0.015	0.40
$4s^24p^3(^2D^\circ)5p$	$^3P_2$	$4s^24p^3(^2P^\circ)5d$	$^3P^\circ_2$	7.54(6)	—	−1.649	−2.228[a]	0.147	0.68
$4s^24p^3(^4S^\circ)5p$	$^3P_2$	$4s^24p^3(^2D^\circ)6s$	$^1D^\circ_2$	3.52(5)	—	−3.087	−3.376[a]	0.005	0.2
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3D_2$	6.90(5)	—	−2.867	−3.162[a]	0.007	0.27
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	8.90(5)	—	−3.032	−2.151[a]	0.005	1.1
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_0$	1.07(7)	—	−2.402	−2.183[a]	0.021	0.68
$4s^24p^3(^2D^\circ)5p$	$^3D_1$	$4s^24p^3(^2P^\circ)6s$	$^3P^\circ_1$	1.29(6)	—	−2.743	−2.690[a]	0.010	0.47
$4s^24p^3(^4S^\circ)5p$	$^5P_2$	$4s^24p^3(^2D^\circ)6s$	$^3D^\circ_3$	5.31(5)	—	−2.832	−2.670[a]	0.007	0.25
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^1D_2$	9.41(5)	—	−2.793	−2.436[a]	0.008	5.1
$4s^24p^3(^4S^\circ)5s$	$^3S^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	2.80(6)	—	−2.321	−2.353[a]	0.024	0.26
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	2.61(5)	—	−3.875	−4.776[a]	0.001	0.17
$4s^24p^3(^4S^\circ)5s$	$^5S^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^1D_2$	3.81(5)	—	−3.275	−4.442[a]	0.002	0.13
$4s^24p^3(^4S^\circ)5p$	$^3P_2$	$4s^24p^3(^2P^\circ)6s$	$^3P^\circ_1$	2.29(6)	—	−2.912	−2.967[a]	0.009	0.098
$4s4p^5$	$^1P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^1D_2$	5.21(5)	—	−1.773	−1.665[a]	0.365	0.60
$4s4p^5$	$^3P^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3F_2$	1.01(5)	—	−3.492	−2.473[a]	0.002	1.3
$4s4p^5$	$^3P^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	1.06(5)	—	−3.449	−2.234[a]	0.002	0.058
$4s4p^5$	$^3P^\circ_0$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	3.21(5)	—	−3.277	−1.639[a]	0.003	14
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3F_3$	3.48(5)	—	−2.868	−2.100[a]	0.008	0.32
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_2$	2.45(5)	—	−3.151	−2.071[a]	0.004	2.1
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^1P_1$	1.04(5)	—	−3.992	−2.533[a]	0.001	0.047
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3D_3$	2.61(5)	—	−3.011	−1.701[a]	0.006	0.27
$4s4p^5$	$^3P^\circ_1$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	7.08(5)	—	−2.967	−1.978[a]	0.006	3.4
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2D^\circ)5p$	$^3P_1$	2.76(6)	—	−2.655	−1.238[a]	0.021	1.3
$4s^24p^4$	$^1S_0$	$4s4p^5$	$^3P^\circ_1$	4.47(7)	—	−1.764	−2.738[a]	0.052	0.56
$4s4p^5$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_0$	3.36(6)	—	−3.432	−2.081[a]	0.005	3.6
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3P_1$	1.05(6)	—	−3.276	−2.036[a]	0.004	1.7
$4s4p^5$	$^3P^\circ_1$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	1.04(6)	—	−2.801	−2.494[a]	0.007	0.40
$4s4p^5$	$^3P^\circ_2$	$4s^24p^3(^2P^\circ)5p$	$^3P_2$	4.53(6)	—	−2.204	−2.840[a]	0.028	0.30
$4s^24p^4$	$^1S_0$	$4s4p^5$	$^1P^\circ_1$	2.89(9)	—	−0.309	−2.385[a]	0.992	1.7
$4s^24p^4$	$^1D_2$	$4s4p^5$	$^1P^\circ_1$	2.60(10)	—	0.350	−0.882[a]	6.924	0.49
$4s^24p^4$	$^3P_0$	$4s4p^5$	$^1P^\circ_1$	7.82(7)	—	−2.010	−2.644[a]	0.017	2.2
$4s^24p^4$	$^3P_2$	$4s4p^5$	$^1P^\circ_1$	6.78(8)	—	−1.316	−3.137[a]	1.360	0.48
$4s^24p^4$	$^3P_0$	$4s^24p^3(^2D^\circ)5s$	$^3D^\circ_1$	7.02(8)	—	−0.880	−1.515[a]	0.280	0.75
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	4.90(8)	—	−1.255	−1.046[a]	0.198	0.74
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	7.34(8)	—	−0.648	−0.657[a]	0.474	0.74
$4s^24p^4$	$^1D_2$	$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	4.89(9)	—	−0.280	0.083[a]	1.816	0.72
$4s^24p^4$	$^3P_0$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_1$	8.82(8)	—	−0.845	−0.894[a]	0.282	0.77
$4s^24p^4$	$^3P_1$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	1.47(9)	—	−1.580	−0.608[a]	0.156	0.81
$4s^24p^4$	$^3P_1$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ_0$	7.95(8)	—	−0.683	−0.029[a]	0.403	0.79
$4s^24p^4$	$^3P_0$	$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	7.80(7)	—	−1.921	−0.521[a]	0.023	0.99
$4s^24p^4$	$^3P_1$	$4s^24p^3(^2P^\circ)5s$	$^1P^\circ_1$	1.06(6)	—	−3.793	−0.691[a]	0.000	0.53

Table 5 (*concluded*).

Lower level		Upper level		A_{ij} (s^{-1}) This work	A_{ij} (s^{-1}) Other works	log(*gf*) This work	log(*gf*) Other work	S_{ij} (a.u.)	Ratio
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ{}_1$	2.48(8)	—	–1.644	0.192^a	0.072	0.86
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2P^\circ)5s$	$^3P^\circ{}_0$	3.88(8)	—	–1.017	0.254^a	0.183	0.86
$4s^24p^4$	$^3P_2$	$4s^24p^3(^2P^\circ)5s$	$^1P^\circ{}_1$	4.57(7)	—	–2.400	–1.245^a	0.012	0.80
Xe III									
$5s^25p^3(^2P)6s$	$^1P^\circ{}_1$	$5s^25p^3(^2P)6p$	$^1D_2$	4.375(7)	10.00(7)^e	–0.262	—	7.379	0.98

Note: The number in brackets represents the power of 10.
^{a}[17].
^{b}[16].
^{c}[12].
^{d}[2].
^{e}[24].

$$f^{\pi k}(\gamma J, \gamma' J') = \frac{1}{\alpha} C_k [\alpha(E_{\gamma' J'} - E_{\gamma J})]^{2k-1} \frac{S^{\pi k}(\gamma J, \gamma' J')}{g_J} \tag{7}$$

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

In calculations we have used the option *extended average level* (EAL) averaging of the expression energy. It is extended to configuration states with not only different total angular momenta but also with different parities. Also, Breit corrections (magnetic interaction between the electrons and retardation effects of the electron–electron interaction), and QED (self-energy and vacuum polarization), and various correlation contributions have been considered. Because of the Coulomb interaction between the electrons, the electron correlation effects are also important, in particular, on fine structure and transitions. Therefore, the configurations including excitations from valence and core have been taken into account (Table 1). QED contributions are self-energy and vacuum polarization, which are also included in the computations of the transition energy. The finite-nucleus effect is taken into account by assuming an extended Fermi distribution for the nucleus. Both the Breit and QED contributions are treated as perturbation and are not included directly in the self-consistent field procedure. The mixing coefficients are calculated by diagonalizing the modified Hamiltonian.

3. Results and discussion

Using GRASP code [32], the calculations of transition parameters such as oscillator strengths, F_{ji}, transition rates (or probabilities), A_{ij} (in s^{-1}), and line strengths, S_{ij} (in a.u.) have been obtained for electric dipole (E1) transitions among levels from configurations selected in Table 1. We have only presented transition parameters for electric dipole (E1) transitions from low-lying levels to ground-state levels in Tables 2, 3, and 4 for Kr III, Xe III, and Rn III, respectively. Only odd-parity states are indicated by the superscript "o" in the tables. Also, the number in brackets represents the power of 10. Electric dipole transitions are calculated in two gauges. The Babushkin gauge can be shown to reduce nonrelativistically to the length form of the matrix element while the Coulomb gauge reduces to the velocity form. We have presented the results here according to the length form. The ratio of velocity and length forms for oscillator strengths have been given in the tables. This ratio must be about 1 for accuracy. We have obtained 62, 454, and 393 energy levels, and 670, 19271, and 18983 electric dipole transitions between these levels performed for Kr III, Xe III, and Rn III, respectively. In Table 2, we have presented transition probabilities, logarithmic values of weighted oscillator strengths, line strengths, and the ratio of velocity and length forms; and compared the logarithmic oscillator strengths with results reported using multiconfigurational Hartree-Fock approach by Raineri et al. [17]. As seen from Table 2, there is good agreement between results, in general. In Tables 3 and 4, we have given the same parameters as in Table 2, except the oscillator strength, F_{ji}, appears instead of logarithmic weighted oscillator strength, log-(F_{ji}), values. There are no values of electric dipole transition parameter for the lines presented in Tables 3 and 4 for Xe III and Rn III, respectively. In Table 5, electric dipole (E1) transition parameters between some high levels for Kr III and only one transition for Xe III have been presented, and compared with those from computational and experimental works [2, 12, 16, 17, 24]. For transition probabilities, our results are mostly in good agreement with results presented by Djenize et al. [2] and Kernahan et al. [12]. There are a few electric dipole transition data for Kr III and Xe III; but there are no data for Rn III in the literature. Most results presented here for these ions, in particular Rn III, are new.

In this work, we have only presented the electric dipole transition parameters from high levels to the levels of ground configuration in Tables 2, 3, and 4. The results in detail have been given as supplementary data[1] for each ion. Atomic data on energy spectrum has great importance in astrophysics and plasma physics applications. Therefore, we hope that the electric dipole transition parameters obtained from this work for doubly ionized krypton, xenon, and radon will be useful for the experimental and theoretical studies in future.

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References

1. J. Ekman, P. Jönsson, S. Gustafsson, H. Hartman, G. Gaigalas, M.R. Godefroid, and C. Froese Fischer. A&A, **564**, A24 (2014). doi:10.1051/0004-6361/201323163.
2. S. Djeniže, V. Milosavljević, and M.S. Dimitrijević. Eur. Phys. J. D, **27**, 209 (2003). doi:10.1140/epjd/e2003-00278-2.
3. R.A. Walch and R.D. Knight. Phys. Rev. A, **38**(5), 2375 (1988). doi:10.1103/PhysRevA.38.2375.
4. E. Träbert, P. Beiersdorfer, G.V. Brown, H. Chen, D.B. Thorn, and E. Biémont. Phys. Rev. A, **64**, 042511 (2001). doi:10.1103/PhysRevA.64.042511.
5. E. Träbert. Phy. Scr. **85**, 048101 (2012). doi:10.1088/0031-8949/85/04/048101.
6. A.G. Calamai and C.E. Johnson. Phys. Rev. **A45**(11), 7792 (1992). doi:10.1103/PhysRevA.45.7792.
7. E. Biémont and J.E. Hansen. Phys. Scr. **34**, 116 (1986). doi:10.1088/0031-8949/34/2/005.
8. F. Bredice, J. Reyna Almandos, M. Gallardo, H.O. Di Rocco, and A.G. Trigueiros. J. Opt. Soc. Am. B, **5**(2), 222 (1988). doi:10.1364/JOSAB.5.000222.

[1]Supplementary data are available with the article through the journal Web site at http://nrcresearchpress.com/doi/suppl/10.1139/cjp-2017-0238.

9. S. Itoi, H. Kai, M. Saito, and Y. Haruyama. Phys. Scr. **T156**, 014023 (2013). doi:10.1088/0031-8949/2013/T156/014023.
10. M. Saito, N. Ojima, S. Itoi, and Y. Haruyama. Phys. Rev. A, **91**, 012508 (2015). doi:10.1103/PhysRevA.91.012508.
11. J.C. Boyce. Phys. Rev. **47**, 718 (1935). doi:10.1103/PhysRev.47.718.
12. J.A. Kernahan, E.H. Pinnington, and W. Ansbacher. J. Opt. Soc. Am B, **4**(7), 1130 (1987). doi:10.1364/JOSAB.4.001130.
13. C.J. Humphreys. Phys. Rev. **47**, 712 (1935). doi:10.1103/PhysRev.47.712.
14. D.E. Osterbrock. Astrophys. J. **114**, 469 (1951).
15. R.H. Garstang. J. Res. Natl. Bur. Stand Sec. A, **68A**(1), 61 (1963). doi:10.6028/jres.068A.004.
16. U. Fink, S. Bashkin, and W.S. Bickel. J. Quant. Spectrosc. Radiat. Transfer, **10**, 1241 (1970). doi:10.1016/0022-4073(70)90008-7.
17. M. Raineri, J.G. Reyna Almandos, F. Bredice, M. Gallardo, A.G. Trigueiros, and S.-G. Pettersson. J. Quant. Spectrosc. Radiat. Transfer, **60**(1), 25 (1998). doi:10.1016/0022-4073(70)90008-7.
18. E.B. Saloman. J. Phys. Chem. Ref. Data, **36**(1), 215 (2007). doi:10.1063/1.2227036.
19. R.J. Peláez, S. Djurović, M. Ćirišan, J.A. Aparicio, and S. Mar. A&A, **539**, A40 (2012). doi:10.1051/0004-6361/201118401.
20. S. Schippers, S. Ricz, T. Buhr, et al. J. Phys. B: At. Mol. Opt. Phys. **47**, 115602 (2014). doi:10.1088/0953-4075/47/11/115602.
21. T. Koizumi, Y. Awaya, A. Fujino, et al. Phys. Scr. **T73**, 131 (1997). doi:10.1088/0031-8949/1997/T73/042.
22. E. Biémont, J.E. Hansen, P. Quinet, and C.J. Zeippen. Astron. Astrophys. Suppl. Ser. **111**, 333 (1995).
23. K.G. Bhushan, H.B. Pedersen, N. Altstein, O. Heber, M.L. Rappaport, and D. Zajfman. Phys. Rev. A, **62**, 012504 (2000). doi:10.1103/PhysRevA.62.012504.
24. H. Sobral, M. Raineri, D. Schinca, M. Gallardo, and R. Duchowicz. IEEE J. Quantum Electron. **35**(9), 1308 (1999). doi:10.1109/3.784590.
25. M. Gallardo, C.A. Massone, A.A. Tagliaferri, and M. Garavaglia. Phys. Scr. **19**, 538 (1979). doi:10.1088/0031-8949/19/5-6/008.
26. P. Bolognesi, S.J. Cavanagh, L. Avaldi, R. Camilloni, M. Zitnik, M. Stuhec, and G.C. King. J. Phys. B: At. Mol. Opt. Phys. **33**, 4723 (2000). doi:10.1088/0953-4075/33/21/316.
27. M. Pernpointner. J. Phys. B: At. Mol. Opt. Phys. **43**, 205102 (2010). doi:10.1088/0953-4075/43/20/205102.
28. P. Andersen, T. Andersen, F. Folkmann, V.K. Ivanov, H. Kjeldsen, and J.B. West. J. Phys. B: At. Mol. Opt. Phys. **34**, 2009 (2001). doi:10.1088/0953-4075/34/10/314.
29. E.B. Saloman. J. Phys. Chem. Ref. Data, **33**(3), 765 (2004). doi:10.1063/1.1649348.
30. E. Biémont and P. Quinet. Phys. Scr. **54**, 36 (1996). doi:10.1088/0031-8949/54/1/006.
31. M. Pernpointner, J.P. Zobel, and N.V. Kryzhevoi. Phys. Rev. A, **85**, 012505 (2012). doi:10.1103/PhysRevA.85.012505.
32. K.G. Dyall, I.P. Grant, C.T. Johnson, F.A. Parpia, and E.P. Plummer. Comp. Phys. Commun. **55**, 425 (1989). doi:10.1016/0010-4655(89)90136-7.
33. I.P. Grant. Relativistic quantum theory of atoms and Molecules. Springer, Verlag, New York. 2007.