

# Energies and E1, M1, E2, and M2 transition rates for states of the $2s^22p^4$ , $2s2p^5$ , and $2p^6$ configurations in oxygen-like ions between F II and Kr XXIX<sup>★</sup>

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## ABSTRACT

Based on relativistic wave functions from multiconfiguration Dirac-Hartree-Fock and configuration interaction calculations, E1, M1, E2, M2 transition rates, weighted oscillator strengths, and lifetimes are evaluated for the states of the  $(1s^2)2s^22p^4$ ,  $2s2p^5$ , and  $2p^6$  configurations in all oxygen-like ions between F II and Kr XXIX. Valence and core-valence correlation effects were accounted for through single-double multireference (SD-MR) expansions to increasing sets of active orbitals. Computed energies are compared with the NIST recommended values, generally differing by less than  $600 \text{ cm}^{-1}$ . For some spectra, significantly larger differences are found and our results are in better agreement with Edlén interpolated values. For levels where experimental lifetimes are available, the agreement is within experimental uncertainty for all but a few lowly ionized spectra. Complete Online tables of energy levels and transition data are available.

**Key words.** atomic data

## 1. Introduction

Transition and energy spectra data of the oxygen isoelectronic sequence are important in astrophysics and plasma physics applications. Accurate atomic data are essential for the interpretation of spectra from various astrophysical sources and in modeling of plasmas. The highly charged ions of iron are important to study because they are a constituent of astrophysical plasmas, especially in high temperature regions. Many researchers have studied O-like ions in the last 25 years. Baluja & Zeippen (1988) calculated excitation energies and transition probabilities for magnetic dipole (M1) and electric quadrupole (E2) transitions within the  $2p^4$  ground-state configuration in the O I isoelectronic sequence for  $Z = 8-36$ , using the CIV3 code. The multiconfiguration Hartree-Fock calculations with relativistic corrections in the Breit-Pauli approximation (MCHF-BP) were performed by Tachiev & Froese Fischer (2002); Froese Fischer & Tachiev (2004) who computed energy and electric dipole (E1), E2, M1, and magnetic quadrupole (M2) transition data between all levels up to  $2p^33d$  for oxygen-like ions in the range  $Z = 8-20$ . Bhatia and Landi performed calculations for several oxygen-like ions such as Ne III (Bhatia et al. 2003) and Ca XIII (Landi & Bhatia 2005). Landi (2005) used the SUPERSTRUCTURE code to obtain energy levels, oscillator strengths, and radiative transition probabilities for all the oxygen-like ions with  $Z = 11-30$ . Deb & Hibbert (2007) presented accurate oscillator strengths, line strengths and radiative rates for 1073 E1 transitions among the 86 levels belonging to the  $2s^22p^4$ ,  $2s2p^5$ ,  $2p^6$ ,

and  $2s^22p^3(4S^o, 2D^o, 2P^o)3l$  configurations in Mg V using the CIV3 code.

Gaigalas et al. (1994) and Vilkas et al. (1994) used the second-order many-body perturbation theory (MBPT) with relativistic corrections in the Breit-Pauli approximation to compute energy spectra, electric dipole, quadrupole and magnetic dipole transitions in the oxygen isoelectronic sequence between the levels of the  $1s^22s^22p^4$ ,  $1s^22s2p^5$  and  $1s^22p^6$  configurations for  $Z = 10-26$ . Froese Fischer et al. (1998) used multiconfiguration Dirac-Hartree-Fock (MCDHF) method to calculate transition rates for the  $2s^22p^4 \ ^3P_{1,2} - 2s^22p^33s \ ^5S_2^o$  and  $2s^22p^4 \ ^3P_{1,2} - 2s2p^5 \ ^3P_2^o$  transitions in the oxygen-like ions for  $Z = 9-18$ . Vilkas et al. (1998, 1999) used multireference Møller-Plesset (MRMP) perturbation theory for the ground and low-lying excited states of oxygen-like iron and oxygen-like ions with nuclear charge up to  $Z = 60$ . No transition data were published. Safronova & Shlyaptseva (1999) used the  $1/Z$  perturbation theory method with inclusion of relativistic and radiative corrections to calculate absolute energies and autoionization rates of the C-, N-, O- and F-like autoionizing doubly-excited states for  $Z = 18-26$ . Bogdanovich et al. used the configuration interaction method to calculate energy spectra for in Mg V, Si VII, and S IX ions (Bogdanovich et al. 1999); energy spectra and lifetimes for all states of first five configurations of Cl X (Bogdanovich et al. 2005); and energy spectra, oscillator strengths and the emission transition probabilities of oxygen-like chromium Cr XVII (Bogdanovich & Karpuškiene 2008).

During the last few years highly ionized ions of iron were of particular interest. Jonauskas et al. (2004) reported 656 energy levels and 214 840 E1, E2 and M1 transition probabilities in oxygen-like Fe XIX using multiconfiguration

<sup>★</sup> Tables 8 and 9 are only available at the CDS via anonymous ftp to [cdsarc.u-strasbg.fr](http://cdsarc.u-strasbg.fr) (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/557/A136>

Dirac-Hartree-Fock (MCDHF). Landi & Gu (2006) produced a large amount of radiative and collisional data for ions of Fe XVII-XXII using the FAC code. Nahar (2011) presented an extensive set of oscillator strengths, line strengths, and radiative decay rates for allowed and forbidden transitions in Fe XIX using the relativistic Breit-Pauli  $\mathbf{R}$ -matrix method.

The present work is motivated by the need to give a full set of consistent and highly accurate transition rates, including E1, E2, M1, M2 multipoles, for levels between the  $2s^22p^4$ ,  $2s2p^5$  and  $2p^6$  configurations for benchmarking. The paper is based on fully relativistic configuration interaction calculations of energies, transition rates, and lifetimes for all ions with  $Z = 9-36$ . The excellent description of the energy separations along the sequence makes it possible to crosscheck experimental energies for a number of ions. The calculations are also helpful in analyzing new data from EBITs, fusion plasmas, and astrophysical sources. The work complements previous work on the  $n = 2$  and  $n = 3$  transitions in the boron, carbon, nitrogen, fluorine and neon sequences (Rynkun et al. 2012a,b; Jönsson et al. 2010, 2011, 2012, 2013a).

## 2. Computational procedure

The multiconfiguration Dirac-Hartree-Fock method (Grant 2007) was used in the present work. Based on the Dirac-Coulomb Hamiltonian

$$H_{\text{DC}} = \sum_{i=1}^N \left( c\alpha_i \cdot p_i + (\beta_i - 1)c^2 + V_i^N \right) + \sum_{i>j}^N \frac{1}{r_{ij}}, \quad (1)$$

where  $V^N$  is the monopole part of the electron-nucleus Coulomb interaction,  $\alpha$  and  $\beta$  the  $4 \times 4$  Dirac matrices, and  $c$  the speed of light in atomic units, the atomic state functions were obtained as linear combinations of symmetry adapted configuration state functions (CSFs)

$$\Psi(\gamma P J M) = \sum_{j=1}^{\text{NCSFs}} c_j \Phi(\gamma_j P J M). \quad (2)$$

Here  $J$  and  $M$  are the angular momentum quantum numbers and  $P$  is parity.  $\gamma_j$  denotes other appropriate labeling of the CSF  $j$ , for example orbital occupancy and coupling scheme. Normally the label  $\gamma$  of the atomic state function is the same as the label of the dominating CSF. The CSFs are built from products of one-electron Dirac orbitals. Based on a weighted energy average of several states, the so called extended optimal level (EOL) scheme (Dyall et al. 1989), both the radial parts of the Dirac orbitals and the expansion coefficients were optimized to self-consistency in the relativistic self-consistent field procedure.

In subsequent relativistic configuration interaction (RCI) calculations the transverse photon interaction (Breit interaction)

$$H_{\text{Breit}} = - \sum_{i<j}^N \left[ \alpha_i \cdot \alpha_j \frac{\cos(\omega_{ij} r_{ij}/c)}{r_{ij}} + (\alpha_i \cdot \nabla_i)(\alpha_j \cdot \nabla_j) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}/c^2} \right] \quad (3)$$

was included in the Hamiltonian. The photon frequencies  $\omega_{ij}$ , used for calculating the matrix elements of the transverse photon interaction, were taken as the difference of the diagonal Lagrange multipliers associated with the Dirac orbitals

(McKenzie et al. 1980). In the RCI calculation the leading quantum electrodynamics corrections, self-interaction and vacuum polarization, were also included.

All calculations were performed with the GRASP2K code (Jönsson et al. 2007). For the calculations of spin-angular parts of matrix elements the second quantization method in coupled tensorial form and quasispin technique (Gaigalas et al. 2001, 1997) were adopted.

All calculations were done in  $jj$ -coupling. The level notations have been converted to  $LSJ$  coupling scheme using the newly developed JJ2LSJ program, part of the latest version of the GRASP2K code by Jönsson et al. (2013b).

## 3. Computation of transition parameters

The evaluation of radiative transition data (transition probabilities, oscillator strengths) between two states  $\gamma'P'J'M'$  and  $\gamma P J M$  built on different and independently optimized orbital sets is non-trivial. The transition data can be expressed in terms of the transition moment which is defined as

$$\langle \Psi(\gamma P J) \| \mathbf{T} \| \Psi(\gamma' P' J') \rangle = \sum_{j,k} c_j c'_k \langle \Phi(\gamma_j P J) \| \mathbf{T} \| \Phi(\gamma'_k P' J') \rangle, \quad (4)$$

where  $\mathbf{T}$  is the transition operator. For electric dipole and quadrupole (E1 and E2) transitions there are two forms of the transition operator, the length (Babushkin) and velocity (Coulomb) forms. For the multiconfiguration Dirac-Hartree-Fock solutions the agreement in the two values may be used as an indicator of accuracy (Froese Fischer 2009). The calculation of the transition moment breaks down to the task of summing up reduced matrix elements between different CSFs. Since the orbitals of the initial and final states are orthonormal but different, the two states  $\gamma'P'J'M'$  and  $\gamma P J M$  were transformed in such a way that the orbital sets became biorthonormal (Olsen et al. 1995). Standard methods were then used to evaluate the matrix elements for the transformed CSFs.

## 4. Generation of configuration expansions

It is often convenient to perform simultaneous calculations in the EOL scheme for states of the same parity occupying roughly the same region in space, as measured by the mean radius of the Dirac-Fock reference orbitals. In the present work simultaneous calculations were performed for the states belonging to the  $2s^22p^4$ ,  $2s2p^5$ , and  $2p^6$ , configurations. The configuration expansions were obtained using the active set method (Sturesson et al. 2007). Here CSFs of a specified parity and  $J$  symmetry are generated by excitations from a number of reference configurations to a set of relativistic orbitals. By applying restrictions on the allowed excitations, different electron correlation effects can be targeted. To monitor the convergence of the calculated energies and transition parameters, the active sets of orbitals were increased in a systematic way by adding layers of correlation orbitals. In the present work, valence and core-valence correlation effects were included.

All expansions were obtained by single and double (SD) excitations from  $1s^22s^22p^4$  and  $1s^22p^6$  for even states and  $1s^22s2p^5$  for odd states to active sets with principal quantum numbers  $n = 3 \dots 8$  and angular symmetries  $s, p, d, f, g, h$  from all shells, with the restriction that there be only a single excitation from the  $1s$  shell. In this way the core-polarization effect of the outer

**Table 1.** Comparison of theoretical energy levels with values derived from observed wavelengths.

Level	$J$	$E_{\text{obs}}^a$	Diff <sub>RCI</sub> <sup>b</sup>	Diff <sub>MRMP</sub> <sup>c</sup>	Diff <sub>MBPT</sub> <sup>d</sup>	Diff <sub>MCHF-BP</sub> <sup>e</sup>	Diff <sub>SS</sub> <sup>f</sup>	Diff <sub>CIV3</sub> <sup>g</sup>
Ne III								
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0
	1	643	2	-15	2	-5	101	-12
	0	921	2	-22	5	-9	148	-18
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	25 841	113	-82	-268	256	3378	894
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	55 753	305	-371	-294	19	16 731	-30
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	204 290	318	345	-3 604	428	11 058	
	1	204 873	327	363	-3597	424	11 135	
	0	205 194	409	345	-3596	423	11 173	
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	289 479	836	2180	-1260	1224	26 032	
Ca XIII								
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0
	1	24 460	8	-80	-251	340	556	-49
	0	28 888	8	-72	-151	-56	600	-319
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	88 208	129	4	80	879	3737	1163
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	178 613	310	-43	-597	30	2074	-393
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	618 268	243	58	-2186	3445	10 265	
	1	638 238	274	129	-2311	3701	10 711	
	0	650 105	309	88	-2386	3884	10 956	
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	850 300	532	189	-3071	4358	19 496	
2p <sup>6</sup> <sup>1</sup> S	0	1 440 320	849	-2361	-6083	5163	34 605	

**Notes.** Energy levels ( $E$ ) and the difference of theoretical energies from observed (Diff.) are given in (cm<sup>-1</sup>).

**References.** <sup>(a)</sup> Kramida et al. (2013); <sup>(b)</sup> present calculations; <sup>(c)</sup> Vilkas et al. (1999); <sup>(d)</sup> Gaigalas et al. (1994); <sup>(e)</sup> Froese Fischer & Tachiev (2012); <sup>(f)</sup> Bhatia et al. (2003); Landi (2005); <sup>(g)</sup> Baluja & Zeippen (1988).

**Table 2.** Comparison of fully relativistic theoretical energy levels with values derived from observed wavelengths for Fe XIX.

Level	$J$	$E_{\text{obs}}^a$	Diff <sub>RCI</sub> <sup>b</sup>	Diff <sub>MRMP</sub> <sup>c</sup>	Diff <sub>PT</sub> <sup>d</sup>	Diff <sub>MBPT</sub> <sup>e</sup>	Diff <sub>FAC</sub> <sup>f</sup>	Diff <sub>MCDP</sub> <sup>g</sup>
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0
	0	75 250	63	-32	150	-508	-52	196
	1	89 441	-7	-190	-1241	-1882	-620	-650
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	168 852	133	-60	-1252	-971	1726	1995
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	325 140	277	-191	-240	-4016	281	1396
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	922 890	154	-35	8010	-5455	6341	10 191
	1	984 740	180	51	8160	-6498	6506	10 266
	0	1 030 020	179	-28	6680	-7267	6038	9672
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	1 267 600	493	171	2200	-8673	15 314	20 173
2p <sup>6</sup> <sup>1</sup> S	0	2 134 180	778	-1370	12 620	-13 969	26 521	41 465

**Notes.** Energy levels ( $E$ ) and the difference of theoretical energies from observed (Diff.) are given in (cm<sup>-1</sup>).

**References.** <sup>(a)</sup> Kramida et al. (2013); <sup>(b)</sup> present calculations; <sup>(c)</sup> Vilkas et al. (1999); <sup>(d)</sup> Safronova & Shlyaptsева (1999); <sup>(e)</sup> Gaigalas et al. (1994); <sup>(f)</sup> Landi & Gu (2006); <sup>(g)</sup> Jonauskas et al. (2004).

2s, 2p on the core is taken into account. Orbitals were optimized simultaneously by layers ( $n$ ) for all levels of the relevant configuration, namely 2s<sup>2</sup>2p<sup>4</sup>, 2s2p<sup>5</sup>, or 2p<sup>6</sup>. The self-consistent field calculations for each layer of orbitals were followed by RCI calculations, including the Breit interaction. At the final stage the configuration expansions from the EOL calculations were augmented by expansions obtained from SD excitations to active sets with  $n = 8$  and angular symmetries  $s, p, d, f, g, h$  to enlarged multireference sets. The multireference set was enlarged to contain all CSFs with with expansion coefficients greater than 0.0114 in the CSF calculation. Particularly important were some configurations with 3d orbitals. For the states of the 1s<sup>2</sup>2s<sup>2</sup>2p<sup>4</sup> and 1s<sup>2</sup>2p<sup>6</sup> configurations, the enlarged multireference set was

{1s<sup>2</sup>2s<sup>2</sup>2p<sup>4</sup>, 1s<sup>2</sup>2p<sup>6</sup>, 1s<sup>2</sup>2s2p<sup>4</sup>3d} whereas for 1s<sup>2</sup>2s2p<sup>5</sup> it was {1s<sup>2</sup>2s2p<sup>5</sup>, 1s<sup>2</sup>2p<sup>5</sup>3d, 1s<sup>2</sup>2s<sup>2</sup>2p<sup>3</sup>3d}. Among the CSFs generated by SD-excitations from the multireference set only those interacting with the multireference states were kept. The leading QED effects – vacuum polarization and self-energy – were included in the final multireference RCI calculations.

The final expansion for the states of the 1s<sup>2</sup>2s<sup>2</sup>2p<sup>4</sup> configuration contained 709 690 CSFs distributed over the  $J = 0, 1, 2$  symmetry blocks. For the states of the 1s<sup>2</sup>2s2p<sup>5</sup> configuration there were 702 892 CSFs distributed over the  $J = 0, 1, 2$  symmetry blocks. Finally, for the  $J = 0$  state of 1s<sup>2</sup>2p<sup>6</sup> configuration there were 67 375 CSFs.

**Table 3.** Comparison of fully relativistic theoretical energy levels with values derived from observed and semi-empirical (SE) wavelengths.

Level	$J$	Obs.(NIST) <sup>a</sup>	SE(Edlén) <sup>b</sup>	Calc. <sup>c</sup>	Diff.(1) <sup>c</sup>	Diff.(2) <sup>c</sup>	Calc. <sup>d</sup>	Diff.(1) <sup>d</sup>	Diff.(2) <sup>d</sup>
Zn XXIII									
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0	0
	0	110 340	110 437	110 316	-24	-121	110 445	105	8
	1	179 060	178 973	178 931	-129	-42	179 045	-15	72
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	267 120	267 325	267 392	272	67	267 408	288	83
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	512 070	512 557	512 589	519	32	512 752	682	195
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	1 176 110	1 176 226	1 176 299	189	73	1 177 520	1410	1294
	1	1 282 970	1 282 957	1 283 062	92	105	1 284 376	1406	1419
	0	1 380 580	1 380 576	1 380 638	58	62	1 381 930	1350	1354
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	1 626 230	1 626 251	1 626 838	608	587	1 627 985	1755	1734
2p <sup>6</sup> <sup>1</sup> S	0	2 697 570	2 697 367	2 698 417	847	1050	2 702 031	4461	4664
Ge XXV									
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0	0
	0	127 240	127 793	127 284	44	-509	127 401	161	-392
	1	243 540	243 568	243 506	-34	-62	243 652	112	84
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	336 200	336 229	336 244	44	15	336 308	108	79
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	646 650	646 933	646 798	148	-135	647 012	362	79
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	1 324 130	1 324 308	1 324 243	113	-65	1 325 473	1343	1165
	1	1 457 310	1 457 440	1 457 479	169	39	1 458 828	1518	1388
	0	1 596 720	1 597 034	1 596 934	214	-100	1 598 310	1590	1276
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	1 842 920	1 842 732	1 843 400	480	668	1 844 637	1717	1905
2p <sup>6</sup> <sup>1</sup> S	0	3 021 850	3 021 332	3 022 627	777	1295	3 026 366	4516	5034
As XXVI									
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0	0
	0	137 320	136 385	135 600	-1720	-785			
	1	281 330	281 802	281 734	404	-68			
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	377 300	376 598	376 586	-714	-12			
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	726 580	726 315	726 071	-509	-244			
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	1 403 750	1 404 724	1 404 572	822	-152			
	1	1 550 530	1 551 663	1 551 701	1171	38			
	0	1 716 190	1 717 549	1 717 342	1152	-207			
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	1 962 370	1 962 613	1 963 325	955	712			
2p <sup>6</sup> <sup>1</sup> S	0		3 195 915	3 197 391		1476			
Se XXVII									
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0	0
	0	147 760	144 941	143 818	-3942	-1123			
	1	323 690	324 396	324 328	638	-68			
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	422 380	421 316	421 279	-1101	-37			
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	814 600	814 628	814 253	-347	-375			
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	1 488 420	1 489 811	1 489 560	1140	-251			
	1	1 649 100	1 650 791	1 650 866	1766	75			
	0	1 845 030	1 847 080	1 846 742	1712	-338			
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	2 090 120	2 091 234	2 091 988	1868	754			
2p <sup>6</sup> <sup>1</sup> S	0		3 379 728	3 381 432		1704			
Br XXVIII									
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0	0
	0	218 800	153 478	151 954	-66 846	-1524	152 035	-66 765	-1443
	1	379 800	371 663	371 606	-8 194	-57	371 858	-7942	195
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	483 040	470 699	470 643	-12 397	-56	470 804	-12 236	105
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0	944 150	912 501	911 968	-32 182	-533	912 282	-31 868	-219
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2		1 579 903	1 579 537		-366	1 580 945		1042
	1		1 755 028	1 755 196		168	1 756 684		1656
	0		1 986 274	1 985 784		-490	1 987 396		1122
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1		2 229 358	2 230 149		791	2 231 636		2278
2p <sup>6</sup> <sup>1</sup> S	0		3 573 416	3 575 415		1999	3 579 486		6070
Kr XXIX									
2s <sup>2</sup> 2p <sup>4</sup> <sup>3</sup> P	2	0	0	0	0	0	0	0	0
	0	160 700	162 011	160 024	-676	-1987	160 088	-612	-1923
	1	423 820	423 933	423 900	80	-33	424 185	365	252
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> D	2	524 890	525 066	525 009	119	-57	525 210	320	144
2s <sup>2</sup> 2p <sup>4</sup> <sup>1</sup> S	0		1 020 595	1 019 865		-730	1 020 232		-363
2s2p <sup>5</sup> <sup>3</sup> P <sup>o</sup>	2	1 674 650	1 675 351	1 674 831	181	-520	1 676 282	1632	931
	1	1 864 320	1 864 603	1 864 921	601	-318	1 866 459	2139	1856
	0	2 133 800	2 135 798	2 135 128	1328	-670	2 136 839	3039	1041
2s2p <sup>5</sup> <sup>1</sup> P <sup>o</sup>	1	2 377 700	2 377 764	2 378 567	867	803	2 380 149	2449	2385
2p <sup>6</sup> <sup>1</sup> S	0		3 777 648	3 779 999		2351	3 784 241		6593

**Notes.** Energy levels ( $E$ ) and the difference of theoretical energies from observed (Diff.(1)) and SE (Diff.(2)) ones are given (in cm<sup>-1</sup>). Primary data source for As XXVI, Se XXVII and Br XXVIII ions at NIST is from Kelly (1987).

**References.** <sup>(a)</sup> Kramida et al. (2013); <sup>(b)</sup> Edlén (1983); <sup>(c)</sup> present calculations; <sup>(d)</sup> Vilkas et al. (1999).

**Table 4.** Comparison of lifetimes.

Ion	State	$\tau_{\text{RCI}}^a$	$\tau_{\text{MCHF-BP}}^b$	$\tau_{\text{exp}}$
F II	$2s^2 2p^4 \ ^1S_0$	397.8	430.22	$420 \pm 12^c$
Ne III	$2s^2 2p^4 \ ^1S_0$	206.5	216.73	$223 \pm 11^d$ $213 \pm 4^e$
Si VII	$2s^2 2p^4 \ ^1D_2$	63.87	63.341	$63.6 \pm 0.7^f$
P VIII	$2s^2 2p^4 \ ^1D_2$	28.69	28.332	$28.63 \pm 0.08^g$
S IX	$2s^2 2p^4 \ ^1D_2$	13.74	13.510	$13.79 \pm 0.05^g$
Ar XI	$2s^2 2p^4 \ ^3P_1$	14.97	14.560	$14.8 \pm 1.1^h$

**Notes.** Lifetimes ( $\tau$ ) is given in (ms).

**References.** <sup>(a)</sup> Present calculations; <sup>(b)</sup> Froese Fischer & Tachiev (2012); <sup>(c)</sup> Calamai et al. (2000); <sup>(d)</sup> Daw et al. (2000); <sup>(e)</sup> Träbert et al. (2001); <sup>(f)</sup> Träbert et al. (1998); <sup>(g)</sup> Träbert et al. (2012); <sup>(h)</sup> Yang et al. (1994).

## 5. Results and evaluation of data

For lower degrees on ionization, the Breit-Pauli (BP) method has often been used in the past. In Table 1, results from three fully relativistic methods based on Dirac theory (RCI, MRMP, MBPT) are compared with Breit-Pauli methods (MCHF-BP, SS, and CIV3). From the differences, we see that in Ne III ( $Z = 10$ ) some of the BP methods are among the most accurate but by Ca XIII ( $Z = 20$ ) the fully relativistic methods that include the Breit and QED corrections have become the most accurate with the present RCI results having the lowest maximum difference with observed. For all levels there is good agreement between RCI and MRMP, except for the highest level. Unlike the present work, many early calculations (MCHF-BP, SS, CIV3, for example) treated the core as inactive. Table 1 shows the importance of the core-polarization correction for levels with a vacancy in the 2s shell. Present results are in much better agreement with observed levels. A very important ion is Fe XIX for which energies have been computed by a variety of relativistic methods, including the recently developed FAC code (Gu 2003). Differences with observed are reported in Table 2. Except for the energy of  $2p^6 \ ^1S$ , the MRMP energies are the most accurate but the RCI values are more regular in their difference with observed.

For ions in the region  $Z > 30$  uncertainties in the “observed” energies become substantial. There are significant discrepancies for As XXVI, Se XXVII and Br XXVIII spectra between the NIST database values based on measurements reported by Kelly (1987) and those derived by Edlén (1983) from a variety of sources. Both are reported in Table 3 and for each method – (c) RCI, and (d) MRMP – the calculated energy level is given along with the differences from the observed values and Edlén values obtained from semiempirically fitted  $1/Z$  expansions. For the  $2s^2 2p^4$  levels in Br XXVIII both theoretical results are in better agreement with the Edlén values.

On the whole, the RCI and MRMP calculations stand out as having the best agreement with observation. Their energy differences are about an order of magnitude smaller than those for other methods.

In Table 4 lifetimes from present calculations are compared with results from MCHF-BP calculations by Fischer and Tachiev and observations. As seen from the table, there is good agreement between theory and experiment for F II and Ne III but for the more highly ionized spectra, the agreement becomes even better. All the computed values are within the uncertainties of experimental measurement.

**Table 5.** Calculated transition energies ( $\Delta E$  in  $\text{cm}^{-1}$ ), type of transition ( $T$ ), weighted oscillator strength ( $gf$ ), transition rate ( $A$  in  $\text{s}^{-1}$ ), and the accuracy ( $R$ ) for E1, E2, M1, M2 transitions in F II.

States		$\Delta E$	$T$	$gf$	$A$	$R$
Upper	Lower	( $\text{cm}^{-1}$ )			( $\text{s}^{-1}$ )	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_2$	165 269	E1	6.646E-01	2.422E+09	1.01
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_2$	165 269	M2	3.254E-10	1.186E+00	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_2$	165 587	E1	2.227E-01	1.357E+09	1.01
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_2$	197 153	E1	2.752E-01	2.378E+09	1.07
$2p^6 \ ^1S_0$	$2s^2 2p^4 \ ^3P_2$	223 908	E2	1.265E-06	4.229E+04	1.05
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_1$	164 926	E1	2.208E-01	8.012E+08	1.01
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_1$	165 243	E1	1.328E-01	8.063E+08	1.01
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^3P_1$	165 528	E1	1.775E-01	3.243E+09	1.01
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_1$	196 810	E1	1.633E-01	1.406E+09	1.07
$2p^6 \ ^1S_0$	$2s^2 2p^4 \ ^3P_1$	223 565	M1	2.661E-10	8.871E+00	
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^3P_0$	165 096	E1	1.769E-01	1.072E+09	1.01
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_0$	196 662	E1	5.558E-02	4.779E+08	1.08
$2s^2 2p^4 \ ^1S_0$	$2s^2 2p^4 \ ^1D_2$	24 279	E2	5.148E-09	2.024E+00	1.29
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^1D_2$	144 285	E1	5.528E-05	1.535E+05	0.88
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^1D_2$	144 603	E1	3.201E-06	1.488E+04	1.31
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^1D_2$	176 169	E1	5.265E-06	3.633E+04	0.97
$2p^6 \ ^1S_0$	$2s^2 2p^4 \ ^1D_2$	202 924	E2	6.423E-11	1.764E+00	0.97
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^1S_0$	120 323	E1	8.476E-06	2.729E+04	0.84
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^1S_0$	151 890	E1	2.325E-07	1.193E+03	0.74
$2p^6 \ ^1S_0$	$2s2p^5 \ ^3P_1^o$	58 321	E1	4.679E-05	1.062E+05	2.06
$2p^6 \ ^1S_0$	$2s2p^5 \ ^1P_1^o$	26 755	E1	3.178E-01	1.517E+08	1.22

Table 5 gives calculated transition energies, weighted oscillator strengths  $gf$ , and transition rates  $A$  in the length gauge. For the electric multipole transitions, the ratio  $R$  between the transition rates in length and velocity gauges is given. A value close to  $R = 1$  for an LS allowed electric multipole transition is a known indicator of accuracy (Froese Fischer 2009). For weak intercombination transitions, the transition amplitude depends sensitively on the mixing of two or more LS terms. Many-body perturbation studies, where calculations are restricted to positive energy states, have shown that there are important contributions to the rate in the velocity gauge from the negative energy continuum whereas rates in the length gauge are relatively unaffected. Variational methods do not explicitly limit the orbitals to have only positive energy components, so for weak intercombination transitions, the usability of  $R$  as an accuracy indicator is somewhat unclear. For the strong E1 transitions the ratio  $R$  is often close to unity. For the intercombination transitions there is a somewhat larger spread for  $R$ . For ions around  $Z = 24$  (Cr XVII) there are internal cancellations in the calculation of the transition moment (Eq. (4)) for the  $2s2p^5 \ ^3P_1^o - 2s^2 2p^4 \ ^1D_2$  transition making the transition rates comparatively low. The internal cancellations affect the two gauges differently, giving ratios  $R$  that differ from 1 by larger amounts. For a discussion about cancellation effects see Ynnerman & Froese Fischer (1995).

Table 6 displays E1, E2, M1 and M2 transition rates from different calculations and NIST critically evaluated data for Mg V. The NIST values are based on Tachiev & Froese Fischer (2002) calculations of line strengths and observed wavelengths and include an accuracy indicator which, for the highest accuracy rating ( $B+$ ) corresponds to an estimated error of  $<7\%$ . The accuracy of our transition rates is similar to the accuracy of the transition energies in Table 1 and, for this moderately ionized atom, there is good agreement between CIV3, MCHF-BP, and RCI.

**Table 6.** Comparison of transition rates in Mg V.

Upper	Lower	Type	$A_{\text{RCI}}^a$	$A_{\text{NIST}}^b$	$A_{\text{MCHF-BP}}^c$	$A_{\text{SS}}^d$	$A_{\text{MBPT}}^e$	$A_{\text{CIV3}}^f$
$2s^2 2p^4 \ ^1D_2$	$2s^2 2p^4 \ ^3P_2$	M1	1.898E+00	1.87E+00 <sup>B</sup>	1.9046E+00	1.798E+00	1.861E+00	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_2$	E1	6.297E+09	6.12E+09 <sup>B+</sup>	6.3532E+09	7.364E+09	5.930E+09	6.292E+09
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_2$	M2	6.632E+00	6.60E+00 <sup>B</sup>	6.6809E+00			
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_2$	E1	3.571E+09	3.46E+09 <sup>B+</sup>	3.5997E+09	4.172E+09	3.356E+09	3.568E+09
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^3P_2$	M2	4.150E+00	4.13E+00 <sup>B</sup>	4.1766E+00	3.792E+00		
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_2$	E1	3.133E+07	3.08E+07 <sup>C</sup>	3.1443E+07	3.285E+07	3.006E+07	
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_2$	M2	3.236E+01	3.22E+01 <sup>B</sup>	3.2874E+01			
$2p^6 \ ^1S_0$	$2s^2 2p^4 \ ^3P_2$	E2	3.820E+02	3.57E+02 <sup>C</sup>	3.6981E+02	3.172E+02	3.514E+02	
$2s^2 2p^4 \ ^1S_0$	$2s^2 2p^4 \ ^3P_1$	M1	2.221E+01	2.15E+01 <sup>B</sup>	2.1971E+01	2.417E+01	2.104E+01	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_1$	E1	2.057E+09	2.00E+09 <sup>B+</sup>	2.0762E+09	2.408E+09	1.941E+09	2.056E+09
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_1$	E1	2.096E+09	2.04E+09 <sup>B+</sup>	2.1145E+09	2.451E+09	1.975E+09	2.094E+09
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_1$	M2	4.330E+00	4.31E+00 <sup>B</sup>	4.3617E+00			
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^3P_1$	E1	8.479E+09	8.23E+09 <sup>B+</sup>	8.5455E+09	9.911E+09	7.975E+09	8.468E+09
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_1$	E1	6.630E+05	5.93E+05 <sup>D</sup>	6.3117E+05	7.129E+05	5.521E+05	6.610E+05
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_1$	M2	1.095E+01	1.09E+01 <sup>B</sup>	1.1119E+01			
$2p^6 \ ^1S_0$	$2s^2 2p^4 \ ^3P_1$	M1	5.564E+00	3.15E+01 <sup>E</sup>	5.7074E+00	6.233E+00	5.737E+00	
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_0$	E1	2.770E+09	2.69E+09 <sup>B+</sup>	2.7942E+09	3.240E+09	2.611E+09	2.767E+09
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_0$	E1	1.212E+06	1.15E+06 <sup>D+</sup>	1.2064E+06	1.382E+06	1.126E+06	1.169E+06
$2s^2 2p^4 \ ^1S_0$	$2s^2 2p^4 \ ^1D_2$	E2	4.195E+00	4.09E+00 <sup>B+</sup>	3.9827E+00	4.329E+00	4.071E+00	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^1D_2$	E1	4.021E+06	4.01E+06 <sup>C</sup>	4.0096E+06	4.558E+06	3.963E+06	4.020E+06
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^1D_2$	M2	1.225E+00	1.22E+00 <sup>B</sup>	1.2313E+00			
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^1D_2$	E1	3.125E+05	2.65E+05 <sup>D</sup>	3.0242E+05	3.496E+05	2.446E+05	3.148E+05
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^1D_2$	M2	2.994E+00	2.98E+00 <sup>B</sup>	3.0059E+00			
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^1D_2$	M2	4.273E+00	4.25E+00 <sup>B</sup>	4.2829E+00	3.897E+00		
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^1D_2$	E1	3.128E+10	3.12E+10 <sup>B+</sup>	3.1711E+10	3.507E+10	3.112E+10	3.130E+10
$2p^6 \ ^1S_0$	$2s^2 2p^4 \ ^1D_2$	E2	2.735E+05	2.74E+05 <sup>B</sup>	2.6967E+05	2.481E+05	2.831E+05	
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^1S_0$	E1	5.981E+05	5.79E+05 <sup>D+</sup>	6.1289E+05	8.450E+05	5.534E+05	6.043E+05
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^1S_0$	E1	1.866E+09	1.89E+09 <sup>B+</sup>	1.8696E+09	1.980E+09	1.929E+09	1.825E+09
$2s2p^5 \ ^1P_1^o$	$2s2p^5 \ ^3P_2^o$	M1	3.428E+00	3.39E+00 <sup>C+</sup>	3.3906E+00	3.250E+00	3.465E+00	
$2p^6 \ ^1S_0$	$2s2p^5 \ ^3P_2^o$	M2	9.131E+01	9.02E+01 <sup>B</sup>	9.2852E+01	7.999E+01		
$2s2p^5 \ ^1P_1^o$	$2s2p^5 \ ^3P_1^o$	M1	1.899E+00	1.95E+00 <sup>C+</sup>	1.9508E+00	1.906E+00	1.992E+00	
$2p^6 \ ^1S_0$	$2s2p^5 \ ^3P_1^o$	E1	7.180E+06	6.58E+06 <sup>D</sup>	7.1894E+06	7.519E+06	5.984E+06	7.202E+06
$2s2p^5 \ ^1P_1^o$	$2s2p^5 \ ^3P_0^o$	M1	2.591E+00	2.54E+00 <sup>C+</sup>	2.5417E+00	2.424E+00	2.595E+00	
$2p^6 \ ^1S_0$	$2s2p^5 \ ^1P_1^o$	E1	2.243E+10	2.20E+10 <sup>B+</sup>	2.2871E+10	2.603E+10	2.149E+10	2.259E+10

**Notes.** Transition probabilities ( $A$ ) are given in ( $s^{-1}$ ). The ratings  $B, B+, C, C+, D, D+, E$  in the  $A_{\text{NIST}}$  column refer to estimated accuracies for transition probabilities.  $B+ : \leq 7\%$ ,  $B : \leq 10\%$ ,  $C+ : \leq 18\%$ ,  $C : \leq 25\%$ ,  $D+ : \leq 40\%$ ,  $D : \leq 50\%$ ,  $E : > 50\%$

**References.** <sup>(a)</sup> Present calculations; <sup>(b)</sup> Kramida et al. (2013); <sup>(c)</sup> Froese Fischer & Tachiev (2012); <sup>(d)</sup> Landi (2005); <sup>(e)</sup> Gaigalas et al. (1994); Vilkas et al. (1994); <sup>(f)</sup> Deb & Hibbert (2007).

Table 7 gives transition rates, including M1 and E2 transitions within the ground configuration, from different calculations and experiment in Fe XIX. Again, the NIST values are based on theoretical calculations for the line strength along with observed wavelengths and, as shown in the table, have a fairly low accuracy rating. The NIST values for E1 transitions in this table are based on Dirac-Hartree-Fock calculations by Cheng et al. (1979), whereas the E2 and M1 transitions are from a SUPERSTRUCTURE calculations (Loulergue et al. 1985). There is good agreement with the BPRM results of Nahar (2011) and the SS results of Landi (2005) who compute the transition rates by using observed wavelengths and only a computed line strength.

The Online Table 8 is similar to Table 1 that reports the calculated and observed energy levels and their difference (in  $\text{cm}^{-1}$ ), the calculated and observed fine-structure splitting

and the difference (in  $\text{cm}^{-1}$ ), as well as the lifetime (in s) of each level for all the spectra from F II – Kr XXIX. Similarly, Table 9 is the Online Version of Table 5 for all the E1, E2, M1, M2 transitions between the levels of the spectra from F II – Kr XXIX.

## 6. Conclusion

In this work, spectroscopic data for the levels of the  $2s^2 2p^4$ ,  $2s2p^5$ , and  $2p^6$  configurations in F II to Kr XXIX are computed using a fully relativistic configuration-interaction method. Our computed energies agree very well with the experimental values, with differences between 300 and 600  $\text{cm}^{-1}$  for the majority of the ions in the sequence. Some possible problems with experimental identification of lines in As XXVI, Se XXVII, and Br XXVIII have been pointed out. The energy levels for these three spectra, presented in this paper, agree much better with the

**Table 7.** Comparison of transition rates in Fe XIX.

Upper	Lower	Type	$A_{\text{RCI}}^a$	$A_{\text{NIST}}^b$	$A_{\text{MCDHF}}^c$	$A_{\text{SS}}^d$	$A_{\text{BPRM}}^e$
$2s^2 2p^4 \ ^3P_1$	$2s^2 2p^4 \ ^3P_2$	M1	1.449E+04	1.45E+04 <sup>C</sup>	1.42E+04		
$2s^2 2p^4 \ ^1D_2$	$2s^2 2p^4 \ ^3P_2$	M1	1.693E+04	1.73E+04 <sup>C</sup>	1.69E+04	1.652E+04	
$2s^2 2p^4 \ ^1D_2$	$2s^2 2p^4 \ ^3P_2$	E2	5.934E+00	6.00E+00 <sup>E</sup>	6.18E+00		
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_2$	E1	3.370E+10	3.9E+10 <sup>C</sup>	3.57E+10	3.492E+10	3.35E+10
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_2$	E1	2.779E+10	3.17E+10 <sup>C</sup>	2.91E+10	2.855E+10	2.77E+10
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_2$	E1	1.099E+10	1.3E+10 <sup>E</sup>	1.15E+10	1.083E+10	1.12E+10
$2s^2 2p^4 \ ^3P_1$	$2s^2 2p^4 \ ^3P_0$	M1	4.046E+01	4.0E+01 <sup>C</sup>		4.117E+01	
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_0$	E1	1.406E+10	1.6E+10 <sup>C</sup>	1.49E+10	1.451E+10	1.40E+10
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_0$	E1	1.248E+09	1.6E+09 <sup>E</sup>	1.34E+09	1.281E+09	1.19E+09
$2s^2 2p^4 \ ^1D_2$	$2s^2 2p^4 \ ^3P_1$	M1	6.605E+02	6.70E+02 <sup>D</sup>	6.99E+02	6.320E+02	
$2s^2 2p^4 \ ^1S_0$	$2s^2 2p^4 \ ^3P_1$	M1	1.398E+05	1.50E+05 <sup>C</sup>	1.39E+05	1.404E+05	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^3P_1$	E1	9.038E+09	1.04E+10 <sup>C</sup>	9.60E+09	9.383E+09	9.02E+09
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^3P_1$	E1	1.094E+10	1.26E+10 <sup>C</sup>	1.16E+10	1.133E+10	1.09E+10
$2s2p^5 \ ^3P_0^o$	$2s^2 2p^4 \ ^3P_1$	E1	5.278E+10	6.05E+10 <sup>C</sup>	5.57E+10	5.445E+10	
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^3P_1$	E1	8.495E+08	9.3E+08 <sup>E</sup>	8.41E+08	8.436E+08	8.57E+08
$2s^2 2p^4 \ ^1S_0$	$2s^2 2p^4 \ ^1D_2$	E2	4.857E+01	4.9E+01 <sup>E</sup>	4.83E+01	4.889E+01	
$2s2p^5 \ ^3P_2^o$	$2s^2 2p^4 \ ^1D_2$	E1	1.912E+09	2.2E+09 <sup>E</sup>	1.94E+09	1.935E+09	1.96E+09
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^1D_2$	E1	1.323E+11	1.49E+11 <sup>C</sup>	1.42E+11		1.32E+11
$2s2p^5 \ ^3P_1^o$	$2s^2 2p^4 \ ^1S_0$	E1	5.970E+08	7.9E+08 <sup>E</sup>	6.35E+08	6.364E+08	5.86E+08
$2s2p^5 \ ^1P_1^o$	$2s^2 2p^4 \ ^1S_0$	E1	9.591E+09	1.1E+10 <sup>C</sup>	1.03E+10	9.798E+09	
$2s2p^5 \ ^3P_0^o$	$2s2p^5 \ ^3P_1^o$	M1	4.841E+03	4.82E+03 <sup>C</sup>		4.853E+03	
$2s2p^5 \ ^1P_1^o$	$2s2p^5 \ ^3P_1^o$	M1	9.250E+03	9.40E+03 <sup>D</sup>		9.173E+03	
$2p^6 \ ^1S_0$	$2s2p^5 \ ^3P_1^o$	E1	1.040E+10	1.2E+10 <sup>E</sup>	1.06E+10	1.026E+10	1.09E+10
$2s2p^5 \ ^1P_1^o$	$2s2p^5 \ ^3P_0^o$	M1	7.722E+03	7.70E+03 <sup>D</sup>		7.462E+03	
$2p^6 \ ^1S_0$	$2s2p^5 \ ^1P_1^o$	E1	1.358E+11	1.61E+11 <sup>C</sup>	1.50E+11	1.403E+11	1.35E+11

**Notes.** Transition probabilities ( $A$ ) are given in ( $s^{-1}$ ). The ratings  $C, D, E$  in the  $A_{\text{NIST}}$  column refer to estimated accuracies for transition probabilities.  $C: \leq 25\%$ ,  $D: \leq 50\%$ ,  $E: > 50\%$

**References.** <sup>(a)</sup> Present calculations; <sup>(b)</sup> Kramida et al. (2013); <sup>(c)</sup> Jonauskas et al. (2004); <sup>(d)</sup> Landi (2005); <sup>(e)</sup> Nahar (2011).

Edlén (1983) values than with NIST databases (results for these ions are based on Kelly 1987). Our energy level calculations are considerably more accurate than other calculations (except for Vilkas and Ishikawa). There are excellent agreements with the most accurate MCHF-BP calculations at the low  $Z$  as well as with experimental lifetimes (Table 4). Basically, the calculations serve as benchmark calculations for transition probabilities for the  $2s^2 2p^4$ ,  $2s2p^5$ , and  $2p^6$  configurations of the oxygen-like sequence without the need for observed transition energies.

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