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Energies, electric dipole (E1), quadrupole (E2), octupole (E3) and magnetic dipole (M1), quadrupole (M2) transition rates for Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX

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Abstract: Energies, weighted oscillator strengths (gf), line strengths (S) and radiative rates (A) for allowed and forbidden transitions are presented for $2s2p^6\ ^2S_{1/2} - 2s^22p^5\ ^2P_{1/2}, ^2P_{3/2}$ and $2s^22p^5\ ^2P_{1/2} - 2s^22p^5\ ^2P_{3/2}$ transitions in fluorine-like Ca XII ($Z = 20$), Ti XIV ($Z = 22$), Cr XVI ($Z = 24$), Fe XVIII ($Z = 26$) and Ni XX ($Z = 28$) ions. Moreover, the allowed electric dipole (E1) and the forbidden electric quadrupole (E2), octupole (E3), magnetic dipole (M1) and quadrupole (M2) transition rates for some transitions are obtained. The $2s^22p^5–2s\ 2p^6$-type transitions of F-like ions are prominent in high-temperature plasmas and are useful for diagnostics. The present results are obtained from configuration interaction atomic structure calculations using the code *SUPERSTRUCTURE* (*SS*) which includes relativistic effects in Breit–Pauli approximation. The comparison of the present energies with the available observed energies displayed very good agreement ($< 1\%$). The presented excitation energy results have been compared with other detailed relativistic approaches such as Dirac–Fock, coupled cluster and configuration interaction for a few ionic states.

1. Introduction

Observations from the several space missions such as Hubble, Chandra and Spitzer provide the lines of highly charged ions. The highly stripped F-like ions are very important for astrophysical applications, high-temperature plasma diagnostics and in laboratory sources [1–3]. The detection of the forbidden transition lines in stellar spectra is very useful to search high-temperature corona for transitions between $2s^22p^5$ and $2s2p^6$ levels. In quasar spectra, such lines are also used to demonstrate the presence of high-temperature plasma associated with these objects. Many forbidden transitions within np^k configurations in F-like ions have identified in tokamak discharges, in the solar corona and flares [4, 5].

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By now, numerous experimental and theoretical studies have been done for fluorine-like ions such as transition energies measured using laser-irradiated solid targets by Reader et al. [6, 7], the energy levels, oscillator strengths and transition probabilities calculated using the multiconfigurational Dirac–Fock (MCDF) method by Cheng et al. [8], transition energies determined using semiempirical method by Edlen [9] and oscillator strengths calculated using CIV3 code by Mohan and Hibbert [10] and Blackford and Hibbert [11]. Moreover, the energy levels and transition rates were calculated using multiconfigurational Breit–Pauli wave functions by Froese Fischer and Tachiev [12]. Jonauskas et al. [13] calculated the energy levels and transition probabilities using the MCDF GRASP code. The relativistic configuration interaction calculations were done for energies, E1, M1, E2 transition rates by Jönsson et al. [14], and the spectral properties such as oscillator strengths, transition probabilities, lifetimes and hyperfine shifts were computed using relativistic coupled cluster method by Nandy and Sahoo [15].

The present paper reports the atomic data for several fluorine-like ions such as Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX having $2p$ open-shell configurations. Energy levels, weighted oscillator strengths, line strengths and transition rates for allowed and forbidden lines have been presented using the SS code [16, 17].

2. Method and formulation

The energies and $\psi = \psi(\gamma SLM_S M_L | r_1, \ldots, r_N)$ wave functions can be obtained by solving time-independent Schrödinger equation for an N-electron system which is given as

$$\left[\sum_{i=1}^{N} \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N} \frac{2}{r_{ij}} \right\} \right] \psi = E\psi; \quad H_{NR}\psi = E\psi \tag{1}$$

where H_{NR} is the nonrelativistic Hamiltonian. While approximate solutions in the nonrelativistic bound-state problems are obtained from Eq. (1), for the ones in the relativistic bound-state problems require the additional Hamiltonian terms.

The computer program $SUPERSTRUCTURE$ and the code's properties which yield bound-state energies in LS coupling and intermediate coupling had been described by Eissner [16, 17]. In this approach, the configuration expansion (CI) wave functions are given by

$$\psi = \sum_i \phi_i c_i \tag{2}$$

where ϕ_i is the configuration basis functions and c_i is the mixing coefficients. In SS, these functions are constructed from one-electron orbitals generated in two-type potential such as both spectroscopic orbitals $P(nl)$ calculated in Thomas–Fermi–Dirac statistical model potential and correlation orbitals $P(\bar{n}l)$ obtained in a Coulomb potential [17–19]

The statistical Thomas–Fermi–Dirac–Amaldi model potential is

$$V^{SM}(r) = \frac{Zeff(\lambda_{nl}, r)}{r} \tag{3}$$

where $Zeff(\lambda_{nl}, r) = Z\left[e^{-Zr/2} + \lambda_{nl}(1 - e^{-Zr/2})\right]\lambda_{nl}$ is the Thomas–Fermi scaling parameters for the orbitals [20].

Since the relativistic effects taken into account through Breit–Pauli (BP) approximation in SS calculations, the relativistic N-electron Breit–Pauli Hamiltonian is given in the form

$$H_{BP} = H_{NR} + H_{rc} \tag{4}$$

where H_{rc} is a sum of relativistic correction operators consisting of one- and two-body parts and may be written as

$$H_{rc} = H_{\text{Mass}} + H_{\text{Dar}} + H_{SO}$$
$$+ \frac{1}{2} \left[g_{ij}(so + so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo') \right] \tag{5}$$

The first three terms in Eq. (5) are the one-body relativistic correction terms: H_{Mass} is the relativistic correction due to the variation of mass with velocity, Darwin term H_{Dar} is the correction term due to the retardation of the electromagnetic field produced by an electron, and H_{SO} is spin–orbit interaction term which is the operator representing spin–orbit interaction of the ith electron in the field of the nucleus [21], and they are given in Eq. (6), respectively [20]

$$H_{\text{Mass}} = -\frac{\alpha^2}{4} \sum_i p_i^4,$$
$$H_{\text{Dar}} = -\frac{\alpha^2}{4} \sum_i \nabla^2 \left(\frac{Z}{r_i}\right), \quad H_{SO} = \alpha^2 \sum_i \frac{Z}{r_i^3} l(i) \cdot s(i) \tag{6}$$

The remaining terms consist of the two-body fine structure terms and the two-body non-fine structure terms. $g_{ij}(so + so')$; spin-other-orbit term and $g_{ij}(ss')$ spin–spin interaction term are the two-body fine structure terms. $g_{ij}(css')$; spin–spin contact interaction term, $g_{ij}(d)$; the two-body Darwin term and $g_{ij}(oo')$; the orbit–orbit interaction term are the two-body non-fine structure terms [16].

The principal physical quantities are determined depending on the line strength. The generalized S line strength for a transition between i and j levels is

$$S^{X\lambda}(i,j) = \left|\langle \Psi_j \| O^{X\lambda} \| \Psi_i \rangle\right|^2, \quad S(ji) = S(ij) \tag{7}$$

where $O^{X\lambda}$ is the appropriate multipole operator. X represents the electric and magnetic type of O operator, and λ refers to a multipolarity [22, 23].

In electric dipole case, transition rate is

$$A_{ji}^{E1} = 2.6773 \times 10^9 (E_j - E_i)^3 \frac{1}{g_j} S^{E1}(i,j) \quad \text{s}^{-1} \tag{8}$$

where $E_{ji} = E_j - E_i$ is the excitation energy. The absorption oscillator strength is

$$f_{ij} = \frac{E_{ji}}{3g_i} S_{ij}, \quad g_i f_{ij} = g_j f_{ji} \tag{9}$$

where energies are expressed in Rydberg and g_i and g_j are the statistical weights of the initial and final states, respectively. Also, the relation between transition rate and oscillator strength is given by the expression

$$A_{ji}.\tau_o = \alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij} \qquad (10)$$

where the time unit is $\tau_o = \hbar/Ry = 4.838 \times 10^{-17}$ s [23, 24].

The electric quadrupole (E2), magnetic dipole (M1), electric octupole (E3) and magnetic quadrupole (M2) radiative transition rates depending on line strengths are

$$A_{ji}^{E2} = 2.6773 \times 10^3 (E_j - E_i)^5 \frac{1}{g_j} S^{E2}(i,j) \quad s^{-1} \qquad (11)$$

$$A_{ji}^{M1} = 3.5644 \times 10^4 (E_j - E_i)^3 \frac{1}{g_j} S^{M1}(i,j) \quad s^{-1} \qquad (12)$$

$$A_{ji}^{E3} = 1.2050 \times 10^{-3} (E_j - E_i)^7 \frac{1}{g_j} S^{E3}(i,j) \quad s^{-1} \qquad (13)$$

$$A_{ji}^{M2} = 2.3727 \times 10^{-2} (E_j - E_i)^5 \frac{1}{g_j} S^{M2}(i,j) \quad s^{-1} \qquad (14)$$

3. Results and discussion

In this work, allowed and forbidden fine structure transitions are studied in fluorine-like Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX ions using the code SS. All calculated energy values for these ions are given by electronic form in Table 1 as supplemental materials. In Table 1, the obtained energies are compared with some experimental data compiled by NIST [25]. These comparisons in Table 1 show that most of the calculated levels are well within < 1% of the observed energies for Ca XII, within 1.3% for Ti XIV, within < 1% for Cr XVI, within < 1% for Fe XVIII and within < 1% for Ni XX. Moreover, the largest discrepancies are 1.2% for the $2p^4 3d$ $^2D_{3/2,5/2}$ levels in Ca XII, 1.8% for the $2p^4 3p$ $^2P_{1/2,3/2}$ levels in Ti XIV, 1.4% for the $2p^4 3d$ $^4P_{5/2}$ levels in Cr XVI, 2.8% for the $2p^4 3d$ $^4P_{3/2,5/2}$ levels in Fe XVIII and 1.3% for the $2p^4 3d$ $^2F_{5/2}$ levels in Ni XX. Therefore, we can say that the overall computed energies are well agreed with the experimental values.

Table 2 presents excitation energies for $2s^2 2p^5$ $^2P_{1/2}$ and $2s 2p^6$ $^2S_{1/2}$ levels obtained with the SS code. These energies are given in Rydberg. The obtained results are compared to some results given in the literature. They agreed very well with those by NIST [25], Jönsson et al. [14] and other results reported using the Dirac–Hartree–Fock (DHF) method and obtained from the CCSD with perturbative treatment of triple excitations CCSD(T) (CCSD; coupled cluster method with single and double excitations) method considering the Dirac–Coulomb (DC), Dirac–Coulomb–Breit (DCB), DCBV (the lower-order vacuum polarization effects incorporating the Uehling and Wichmann-Kroll potentials along with DCB) and DCBVS (the lowest-order self-energy correction to the DCBV) Hamiltonians given by Nandy and Sahoo [15]. Most of the NIST data include the results of

Table 1 Energy levels (Ry) for (a) Ca XII, (b) Ti XIV, (c) Cr XVI, (d) Fe XVIII and (e) Ni XX

Config. number	Configuration	Term	J	E^{SS}	E^{NIST}
(a)					
1	$2s^2 2p^5$	$^2P^\circ$	3/2	0	0
1			1/2	0.2737	0.2737
2	$2s 2p^6$	^2S	1/2	6.461	6.461
3	$2s^2 2p^4(^3P)3s$	^4P	5/2	28.045	27.906
3			3/2	28.167	28.041
3	$2s^2 2p^4(^3P)3s$	^2P	1/2	28.270	28.152
3			3/2	28.340	28.229
3	$2s^2 2p^4(^1D)3s$	^2D	1/2	28.480	28.384
3			5/2	28.905	28.782
3	$2s^2 2p^4(^1S)3s$	^2S	3/2	28.911	28.79
6	$2s^2 2p^4(^3P)3d$	^4P	1/2	29.619	29.613
6			1/2	31.883	31.674
6			3/2	31.940	31.708
6	$2s^2 2p^4(^3P)3d$	^4F	5/2	32.019	31.798
6	$2s^2 2p^4(^3P)3d$	^2P	5/2	31.917	31.712
6			1/2	31.987	31.773
6	$2s^2 2p^4(^3P)3d$	^2D	3/2	32.189	31.969
6			3/2	32.081	31.845
6	$2s^2 2p^4(^3P)3d$	^2F	5/2	32.243	31.999
6	$2s^2 2p^4(^1D)3d$	^2S	5/2	32.089	31.848
6	$2s^2 2p^4(^1D)3d$	^2F	1/2	32.692	32.435
6	$2s^2 2p^4(^1D)3d$	^2D	5/2	32.694	32.467
6			5/2	32.243	32.577
6	$2s^2 2p^4(^1D)3d$	^2P	3/2	32.081	32.668
6	$2s^2 2p^4(^1S)3d$	^2D	3/2	32.189	32.577
6			5/2	33.650	33.242
16	$2s 2p^5(^3P^\circ)3s$	$^2P^\circ$	3/2	32.974	33.282
16			3/2	34.133	34.063
	$2s^2 2p^5$	$^2P^\circ$	1/2	34.286	34.226
(b)					
1	$2s^2 2p^5$	$^2P^\circ$	3/2	0	0.00000
1			1/2	0.430307	0.43029
2	$2s 2p^6$	^2S	1/2	7.56258	7.47031
3	$2s^2 2p^4(^3P)3s$	^4P	5/2	36.7471	36.40662
3			3/2	36.9201	36.58687
3			1/2	36.99811	36.7798
3	$2s^2 2p^4(^3P)3s$	^2P	3/2	37.18655	36.8464
3			1/2	37.63268	37.0498
3	$2s^2 2p^4(^1D)3s$	^2D	5/2	37.64474	37.478
3			3/2	38.29952	37.49021
5	$2s^2 2p^4(^3P)3p$	$^4P^\circ$	5/2	38.31211	38.11543
5			3/2	38.44815	38.1259
5			1/2	38.50655	38.2740
5	$2s^2 2p^4(^3P)3p$	$^4D^\circ$	7/2	38.56637	38.3269
5			5/2	38.7278	38.36803
5			3/2	38.79661	38.5663

Table 1 continued

Config. number	Configuration	Term	J	E^{SS}	E^{NIST}
5			1/2	38.85878	38.6137
3	$2s^22p^4(^1S)3s$	^2S	1/2	38.5197	38.466
5	$2s^22p^4(^3P)3p$	$^2P°$	1/2	38.7526	38.5423
5			3/2	38.97527	38.6743
5	$2s^22p^4(^3P)3p$	$^2D°$	5/2	38.86455	38.68251
5			3/2	39.03456	38.8643
5	$2s^22p^4(^3P)3p$	$^4S°$	3/2	39.40343	38.7940
5	$2s^22p^4(^3P)3p$	$^2S°$	1/2	39.04287	38.8571
5	$2s^22p^4(^1D)3p$	$^2F°$	5/2	39.47704	39.2131
5			7/2	39.63661	39.2957
5	$2s^22p^4(^1D)3p$	$^2D°$	3/2	39.68574	39.4507
5			5/2	40.15311	39.5027
5	$2s^22p^4(^1D)3p$	$^2P°$	3/2	40.25205	39.90106
5	$2s^22p^4(^1S)3p$	$^2P°$	3/2	40.75559	40.3985
5			1/2	40.86491	40.4881
6	$2s^22p^4(^3P)3d$	^4D	7/2	40.6686	40.4610
6			5/2	40.70292	40.470
6			3/2	40.75519	40.50933
6			1/2	40.83401	40.5670
6	$2s^22p^4(^3P)3d$	^4F	9/2	40.94615	40.6503
6			7/2	41.01778	40.73241
6			5/2	41.15384	40.90673
6			3/2	41.19113	40.99222
6	$2s^22p^4(^3P)3d$	^4P	1/2	41.10139	40.81896
6			3/2	41.10417	40.902
6			5/2	41.26551	41.021
6	$2s^22p^4(^3P)3d$	^2P	1/2	41.18808	40.960
6			3/2	41.49438	41.236
6	$2s^22p^4(^3P)3d$	^2F	7/2	42.14633	40.9902
6			5/2	42.02777	41.11705
6	$2s^22p^4(^3P)3d$	^2D	3/2	41.31567	41.066
6			5/2	41.75617	41.298
6	$2s^22p^4(^1D)3d$	^2G	7/2	41.77071	41.5587
			9/2	41.95383	41.56786
6	$2s^22p^4(^1D)3d$	^2S	1/2	41.98146	41.76
6	$2s^22p^4(^1D)3d$	^2F	5/2	42.02777	41.7731
			7/2	42.14633	41.8260
6	$2s^22p^4(^1D)3d$	^2P	3/2	42.16627	41.92205
6	$2s^22p^4(^1D)3d$	^2D	5/2	42.29234	41.94802
			3/2	42.2928	42.077
6	$2s^22p^4(^1S)3d$	^2D	5/2	43.15206	42.700
			3/2	43.23661	42.77
16	$2s2p^5(^3P°)3s$	$^2P°$	3/2	44.01267	43.546
			1/2	44.85627	43.796
(c)					
1	$2s^22p^5$	$^2P°$	3/2	0	0.00000
1			1/2	0.64604	0.64602

Table 1 continued

Config. number	Configuration	Term	J	E^{SS}	E^{NIST}
2	$2s2p^6$	^2S	1/2	8.54576	8.5458
3	$2s^22p^4(^3P)3s$	^4P	5/2	46.537	46.007
3			3/2	46.7707	46.222
3			1/2	47.0336	46.559
3	$2s^22p^4(^3P)3s$	^2P	3/2	47.148	46.640
3			1/2	47.3884	46.870
3	$2s^22p^4(^1D)3s$	^2D	5/2	47.846	47.327
3			3/2	47.8705	47.350
3	$2s^22p^4(^1S)3s$	^2S	1/2	48.9196	48.511
6	$2s^22p^4(^3P)3d$	^4P	1/2	51.6667	51.100
6			3/2	51.7832	51.219
6			5/2	52.1206	51.397
6	$2s^22p^4(^3P)3d$	^4F	5/2	51.8168	51.238
6	$2s^22p^4(^3P)3d$	^2P	1/2	51.8612	51.291
6			3/2	52.2388	51.680
6	$2s^22p^4(^3P)3d$	^2D	3/2	52.0146	51.469
6			5/2	52.3344	51.767
6	$2s^22p^4(^3P)3d$	^2F	5/2	51.9653	51.57
6	$2s^22p^4(^1D)3d$	^2S	1/2	52.8226	52.258
6	$2s^22p^4(^1D)3d$	^2P	3/2	53.0769	52.454
6	$2s^22p^4(^1D)3d$	^2D	5/2	53.1018	52.463
6			3/2	53.2738	52.676
6	$2s^22p^4(^1S)3d$	^2D	5/2	54.1376	53.375
6			3/2	54.2467	53.497
16	$2s2p^5(^3P°)3s$	$^2P°$	3/2	54.5008	54.222
16			1/2	54.8431	54.554
(d)					
1	$2s^22p^5$	$^2P°$	3/2	0.0	0.0
1			1/2	0.9347	0.9348
2	$2s2p^6$	^2S	1/2	9.70	9.70
3	$2s^22p^4(^3P)3s$	^4P	5/2	57.21	56.70
3			1/2	57.50	57.50
3			3/2	57.88	57.57
3	$2s^22p^4(^3P)3s$	^2P	3/2	57.50	56.94
3			1/2	58.35	57.80
3	$2s^22p^4(^1D)3s$	^2D	5/2	58.83	58.32
3			3/2	58.87	58.36
3	$2s^22p^4(^1S)3s$	^2S	1/2	60.16	59.92
6	$2s^22p^4(^3P)3d$	^4P	1/2	63.94	62.50
6			3/2	64.46	62.63
6			5/2	64.62	62.91
6	$2s^22p^4(^3P)3d$	^2F	5/2	64.17	62.70
6	$2s^22p^4(^3P)3d$	^4D	1/2	63.58	62.91
6			3/2	63.49	63.05
6	$2s^22p^4(^3P)3d$	^2P	3/2	64.74	63.31
6	$2s^22p^4(^3P)3d$	^2D	5/2	64.09	63.40
6	$2s^22p^4(^1D)3d$	^2S	1/2	65.97	63.92

Table 1 continued

Config. number	Configuration	Term	J	E^{SS}	E^{NIST}
6	$2s^2 2p^4(^1D)3d$	^2P	3/2	66.38	64.14
6			1/2	66.86	64.46
6	$2s^2 2p^4(^1D)3d$	^2D	5/2	65.37	64.16
6			3/2	64.09	64.39
6	$2s^2 2p^4(^1S)3d$	^2D	5/2	65.64	65.31
6			3/2	65.69	65.47
16	$2s2p^5(^3P°)3s$	$^4P°$	5/2	65.56	65.48
16			3/2	65.88	65.59
			1/2	66.28	65.84
16	$2s2p^5(^3P°)3s$	$^2P°$	3/2	66.38	66.08
17	$2s2p^5(^3P°)3p$	^4D	3/2	68.21	68.02
17	$2s2p^5(^3P°)3p$	^2D	5/2	68.33	68.14
17			3/2	69.16	68.96
16	$2s2p^5(^3P°)3p$	^2P	3/2	68.91	68.23
16			1/2	68.96	68.42
17	$2s2p^5(^3P°)3p$	^4P	5/2	68.74	68.42
17			3/2	68.77	68.62
	$2s2p^5(^3P°)3p$	^2S	1/2	69.38	69.25
	$2s2p^5(^1P°)3p$	^2D	3/2	71.17	70.75
17			5/2	71.37	70.93
17	$2s2p^5(^1P°)3p$	^2P	1/2	71.41	70.95
17			3/2	71.51	71.03
(e)					
1	$2s^2 2p^5$	$^2P°$	3/2	0	0.00000
1			1/2	1.31185	1.31185
2	$2s2p^6$	^2S	1/2	10.955	10.955
3	$2s^2 2p^4(^3P)3s$	^4P	5/2	68.971	68.470
3			1/2	69.830	69.377
3			3/2	69.288	69.696
3	$2s^2 2p^4(^3P)3s$	^2P	3/2	69.288	68.744
3			1/2	70.426	69.923
3	$2s^2 2p^4(^1D)3s$	^2D	5/2	70.976	70.493
3			3/2	71.031	70.552
5	$2s^2 2p^4(^3P)3p$	$^4D°$	7/2	71.956	71.384
5			3/2	72.571	71.982
5			5/2	73.021	72.325
5	$2s^2 2p^4(^3P)3p$	$^2D°$	5/2	71.940	71.568
5	$2s^2 2p^4(^3P)3p$	$^4P°$	5/2	71.547	
			1/2	71.870	72.271
3	$2s^2 2p^4(^1S)3s$	^2S	1/2	72.639	72.44
5	$2s^2 2p^4(^1D)3p$	$^2F°$	5/2	73.505	73.044
5			7/2	73.825	73.289
5	$2s^2 2p^4(^1D)3p$	$^2D°$	5/2	73.287	73.558
6	$2s^2 2p^4(^3P)3d$	^4F	9/2	75.335	74.691
6			5/2	75.906	75.34
6			7/2	76.3766	75.749
6	$2s^2 2p^4(^3P)3d$	^2F	7/2	75.428	74.853
6			5/2	76.213	75.23

Table 1 continued

Config. number	Configuration	Term	J	E^{SS}	E^{NIST}
6	$2s^2 2p^4(^3P)3d$	^4P	1/2	75.608	74.96
6			3/2	75.788	75.12
6	$2s^2 2p^4(^3P)3d$	^4D	7/2	76.376	
6			3/2	76.169	75.90
6	$2s^2 2p^4(^3P)3d$	^2P	3/2	76.7136	76.12
6	$2s^2 2p^4(^3P)3d$	^2D	5/2	76.81	76.2
6	$2s^2 2p^4(^1D)3d$	^2G	7/2	77.084	76.542
6	$2s^2 2p^4(^1D)3d$	^2S	1/2	77.37	76.76
6	$2s^2 2p^4(^1D)3d$	^2F	7/2	77.504	76.895
6	$2s^2 2p^4(^1D)3d$	^2P	3/2	77.646	76.96
			1/2	78.084	77.41
6	$2s^2 2p^4(^1D)3d$	^2D	5/2	77.712	77.02
6			3/2	77.998	77.31
6	$2s^2 2p^4(^1S)3d$	^2D	3/2	79.462	78.68
17	$2s2p^5(^3P°)3p$	^2D	5/2	82.138	81.18
17			3/2	82.755	82.49
17	$2s2p^5(^3P°)3p$	^4D	3/2	81.402	81.18
17	$2s2p^5(^3P°)3p$	^2P	3/2	81.839	81.67
17			1/2	82.021	81.81
17	$2s2p^5(^3P°)3p$	^4P	3/2	82.184	82.09
17	$2s2p^5(^3P°)3p$	^2S	1/2	82.916	82.85
17	$2s2p^5(^1P°)3p$	^2D	3/2	84.685	84.3
17			5/2	85.035	84.59
17	$2s2p^5(^1P°)3p$	^2P	1/2	85.031	84.64
17			3/2	85.190	84.78
7	$2s^2 2p^4(^3P)4s$	^2P	3/2	93.531	92.79
7	$2s^2 2p^4(^3P)4s$	^4P	3/2	94.549	94.02
	$2s^2 2p^4(^3P)4d$	^2D	5/2	94.595	95.34
9	$2s^2 2p^4(^3P)4d$	^4F	5/2	96.089	96.0
9			3/2	96.686	96.0
9	$2s^2 2p^4(^3P)4d$	^4P	5/2	95.756	96.38
9	$2s^2 2p^4(^3P)4d$	^2P	3/2	96.924	96.42
9	$2s^2 2p^4(^1D)4d$	^2D	5/2	97.049	97.10
9			3/2	97.101	97.27
9	$2s^2 2p^4(^1D)4d$	^2S	1/2	97.769	97.10
9	$2s^2 2p^4(^1D)4d$	^2F	5/2	97.761	97.30
9	$2s^2 2p^4(^1S)4d$	^2D	3/2	99.719	98.90

Sugar and Corlis [26], Sugar and Musgrove [27–29], and Shirai et al. [30] obtained either from the tokamak plasma experiments or from the Dirac–Fock calculations.

We presented the line strengths, oscillator strengths and transition rates of the first two excited states for some F-like ions in Table 3. The line strengths (S) were given for both the allowed E1 and forbidden M1 and E2 transitions. Also, in same table, we evaluated the transition rates and given the weighted oscillator strengths. We compared our

Table 2 Excitation energies (in Ry) for some F-like ions obtained with the SUPERSTRUCTURE code

Ions	This Work SS	Kramida et al. [25]	Jönsson et al. [14]	Nandy and Sahoo [15]			
				DC	DCB	DCBV	DCBVS
Ca XII							
$2s^22p^5$ $^2P_{3/2}$	0.0	0.0	0.0				
$2s^22p^5$ $^2P_{1/2}$	0.274124	0.274097	0.274191				
$2s2p^6$ $^2S_{1/2}$	6.469717	6.469252	6.472679				
Ti XIV							
$2s^22p^5$ $^2P_{3/2}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$2s^22p^5$ $^2P_{1/2}$	0.430812	0.43083	0.430777	0.443125	0.430086	0.430083	0.431062
$2s2p^6$ $^2S_{1/2}$	7.485995	7.476934	7.486043	7.494727	7.494569	7.494889	7.494881
Cr XVI							
$2s^22p^5$ $^2P_{3/2}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$2s^22p^5$ $^2P_{1/2}$	0.646843	0.646825	0.646766	0.663504	0.645647	0.645644	0.647875
$2s2p^6$ $^2S_{1/2}$	8.556469	8.553741	8.562196	8.571693	8.571873	8.580975	8.5811
Fe XVIII							
$2s^22p^5$ $^2P_{3/2}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$2s^22p^5$ $^2P_{1/2}$	0.935931	0.935027	0.934951	0.953402	0.935093	0.935089	0.935005
$2s2p^6$ $^2S_{1/2}$	9.714425	9.714434	9.715859	9.738228	9.742777	9.745331	9.752225
Ni XX							
$2s^22p^5$ $^2P_{3/2}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$2s^22p^5$ $^2P_{1/2}$	1.313495	1.313495	1.308806	1.345581	1.309149	1.309143	1.318372
$2s2p^6$ $^2S_{1/2}$	10.96901	10.96898	10.97065	11.00286	11.00946	11.01298	11.02631

transition rate results with the other calculations: Jönsson et al. [14], Tachiev and Fischer [12], Kaufman and Sugar [31] and Nandy and Sahoo [15]. It was seen that our transition probability results differ from those by Jönsson et al. [14] with 4–6% for E1 transitions, with 0.2–4% for M1 transitions and with 0.8–3% for E2 transitions, from those by Tachiev and Fischer [12] with 4–5% for E1 transitions, with 3% for E2 transitions, with 2–5% for M1 transitions, from those by Kaufman and Sugar [31] with 2–4% for M1 transitions and from those by Nandy and Sahoo [15], with 5–7% for E1 transitions, with 2–3% for E2 transitions and with 2–8% for M1 transitions. Moreover, some radiative E3 and M2 decay rates for the forbidden transitions of relevant F-like ions are given in Table 4 as new data for these ions. In Table 4, (i, j) is the level numbers, (C_i, C_j) is configuration indices: $2s^22p^5(1)$, $2s2p^6(2)$, $2s^22p^43s(3)$, $2s^22p^43p(5)$, $2s^22p^43d(6)$, $2s^22p^44s(7)$, $2s^22p^44p(8)$, $2s^22p^44d(9)$, $2s^22p^44f(10)$ and $2s2p^53s(11)$, and T denotes the LS term. Moreover, g_i and g_j are the statistical weights of the lower and upper levels, and E_i and E_j are the energies in Rydberg unit of the lower

and upper levels, respectively. It is seen from all comparisons that the present results have good agreement with other results for the same spin-dipole transitions.

4. Conclusions

We determined energy levels, excitation energies, weighted oscillator strengths and transition rates using *SS* code for some considered F-like highly charged ions. The determined quantities were compared with available results from the literature. For energies, very good agreements were obtained with those of the measured levels. The average agreement of energies is within < 1%. Also, E1, E2 and M1 transition rates are in very good agreement with the earlier data given in the literature.

We expect that the obtained atomic properties such as radiative decay rates and weighted oscillator strengths are enough accurate data and very useful for the astrophysical plasma analysis.

Table 3 Line strengths (S_{ik} in au), weighted oscillator strengths (gf) and transition rates (A in s^{-1}), for the considered ions

			S_{ik}	$g_i f_{ik}$	A_{ki}	Jönsson et al. [14]	Tachiev and Fischer [12]	Kaufman and Sugar [31]	Nandy and Sahoo [15]
Ca XII									
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{1/2}$	E1	0.120412	2.594e−01	4.349e+10	4.146e+10	4.167e+10		
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E1	0.059892	1.235e−01	1.900e+10	1.803e+10	1.810e+10		
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	M1	1.33		1.619e−02	1.547e−02	1.6285e−02		
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E2	7.876e−03		4.875e+02	4.871e+02	5.0376e+02		
Ti XIV									
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{1/2}$	E1	0.048847	1.147e−01	2.285e+10	2.136e+10	2.151e+10		2.141e+10
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E1	0.098218	2.447e−01	5.49e+10	5.163e+10	5.212e+10		5.097e+10
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	M1	1.333		1.839e+03	1.888e+03	1.976e+03	1.890 e+03	1.881e+03
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E2	4.768e−03		9.467e−02	9.124e−02	9.793e−02		9.110e−02
Cr XVI									
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{1/2}$	E1	0.40309	1.061e−01	2.660e+10	2.476e+10			2.481e+10
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E1	0.081178	2.312e−01	6.782e+10	6.358e+10			6.29e+10
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	M1	1.333		6.403e+03	6.386e+03		6.390e+03	6.341e+03
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E2	3.084e−03		4.639e−01	4.518e−01			4.512e−01
Fe XVIII									
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{1/2}$	E1	0.033822	9.884e−02	3.051e+10	2.824e+10			2.826e+10
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E1	0.068209	2.206e−01	8.340e+10	7.784e+10			7.715e+10
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	M1	1.332		1.939e+04	1.933e+04		1.930e+04	1.923e+04
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E2	2.080e−03		1.984e+00	1.939e+00			1.937e+00
Ni XX									
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{1/2}$	E1	0.028079	9.031e−02	3.373e+10	3.181e+10			3.180e+10
$2s\,2p^6$ $^2S_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E1	0.056779	2.075e−01	1.00e+11	9.512e+10			9.441e+10
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	M1	1.332		5.359e+04	5.340e+04		5.342e+04	5.315e+04
$2s^2 2p^5$ $^2P_{1/2}$	$2s^2 2p^5$ $^2P_{3/2}$	E2	1.455e−03		7.55e+00	7.386e+00			7.387e+00

Table 4 Transition probabilities A_{ji} (s^{-1}) for the forbidden electric octupole (E3) and magnetic quadrupole (M2) transitions in relevant F-like ions such as (a) Ca XII, (b) Ti XIV, (c) Cr XVI, (d) Fe XVIII and (e) Ni XX

i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	A_{ji}	
						E3	M2
(a)							
2–4	2P$_0$ 1–4P$_e$ 3	2–6	25.21513	2.7377E−01	28.045E+00	2.349E+02	3.470E+03
2–9	2P$_0$ 1–2D$_e$ 3	2–6	24.49662	2.7377E−01	28.905E+00	1.463E+04	1.555E+04
3–11	2S$_e$ 2–4P$_O$ 5	2–6	29.65592	6.4616E+00	29.572E+00	2.178E−02	9.551E+00
6–11	4P$_e$ 3–4P$_0$ 5	2–6	665.1585	28.270E+00	29.572E+00	8.050E−06	2.69E−02
8–11	2P$_e$ 3–4P$_0$ 5	2–6	820.9614	28.480E+00	29.572E+00	8.770E−09	2.661E−02
4–14	4P$_e$ 3–4P$_0$ 5	6–2	472.1591	28.045E+00	29.675E+00	1.316E−04	1.108E−01
9–14	2D$_e$ 3–4P$_0$ 5	6–2	23.93681	28.905E+00	29.675E+00	9.150E−07	1.89E−03
3–15	2S$_e$ 2–4D$_0$ 5	2–8	29.4451	6.4616E+00	29.765E+00	1.219E+00	0.00E+00
5–15	4P$_e$ 3–4D$_0$ 5	4–8	514.8402	28.167E+00	29.765E+00	1.686E−03	3.158E−03
6–15	4P$_e$ 3–4D$_0$ 5	2–8	573.124	28.270E+00	29.765E+00	1.114E−03	0.00E+00
7–15	2P$_e$ 3–4D$_0$ 5	4–8	599.5178	28.340E+00	29.765E+00	2.397E−04	3.174E−01
8–15	2P$_e$ 3–4D$_0$ 5	2–8	685.1632	28.480E+00	29.765E+00	1.926E−06	0.00E+00
10–15	2D$_e$ 3–4D$_0$ 5	4–8	1047.433	28.911E+00	29.765E+00	1.484E−07	2.719E−03
13–15	4P$_e$ 5–4D$_0$ 5	2–6	13018.1	29.619E+00	29.765E+00	2.204E−12	0.00E+00
6–16	4P$_e$ 3–4D$_0$ 5	2–8	555.6507	28.270E+00	29.812E+00	9.807E−05	5.144E−02
8–16	2P$_e$ 3–4D$_0$ 5	2–6	660.3385	28.480E+00	29.812E+00	3.621E−04	7.369E−02
(b)							
2–4	2P$_0$ 1–4P$_e$ 3	2–6	36570	4.303E−01	3.657E+04	1.137E+03	7.652E+03
2–9	2P$_0$ 1–2D$_e$ 3	2–6	37.63	4.303E−01	3.763E+01	4.254E+04	4.346E+04
3–11	2S$_e$ 2–4P$_O$ 5	2–6	30.728	7.562E+00	3.829E+01	1.73E−01	1.441E+01
6–11	4P$_e$ 3–4P$_0$ 5	2–6	1.37	3.692E+01	3.829E+01	8.048E−06	3.351E−02
8–11	2P$_e$ 3–4P$_0$ 5	2–6	1.11	3.718E+01	3.829E+01	2.143E−08	2.363E−02
4–13	4P$_e$ 3–4P$_0$ 3	6–2	36531.5	3.657E+04	3.844E+01	2.349E−04	1.138E−01
9–13	2D$_e$ 3–4P$_0$ 3	6–2	0.87	3.763E+01	3.844E+01	1.402E−06	3.714E−03
11–14	4P$_o$ 5–2 S$_e$ 3	6–2	0.21	3.829E+01	3.850E+01	2.115E−12	1.392E−06
3–15	2S$_e$ 2–4D$_0$ 5	2–8	30.948	7.562E+00	3.851E+01	4.112E+00	0
5–15	4P$_e$ 3–4D$_0$ 5	4–8	1.77	3.674E+01	3.851E+01	1.335E−03	2.504E−02
6–15	4P$_e$ 3–4D$_0$ 5	2–8	1.59	3.692E+01	3.851E+01	7.942E−04	0
7–15	2P$_e$ 3–4D$_0$ 5	4–8	1.52	3.699E +01	3.851E+01	2.571E−04	3.037E−01
8–15	2P$_e$ 3–4D$_0$ 5	2–8	1.33	3.718E+01	3.851E+01	9.352E−08	0
10–15	2D$_e$ 3–4D$_0$ 5	4–8	0.87	3.764E+01	3.851E+01	1.401E−07	3.853E−03
14–15	2 S$_e$ 3–4D$_0$ 5	2–6	0.07	3.8506E+01	3.851E+01	8.808E−20	0
3–16	2S$_e$ 2–4D$_0$ 5	2–6	30.998	7.562E+00	3.856E+01	5.141E+00	8.868E+01
6–16	4P$_e$ 3–4D$_0$ 5	2–8	1.64	3.692E+01	3.856E+01	5.350E−05	4.717E−02
8–16	2P$_e$ 3–4D$_0$ 5	2–6	1.38	3.718E+01	3.856E+01	2.531E−04	4.965E−02
14–16	2 S$_e$ 3–4D$_0$ 5	2–6	0.12	3.8506E+01	3.856E+01	4.247E−15	9.457E−10
(c)							
2–4	2P$_0$ 1–4P$_e$ 3	2–6	2.52E+01	6.4603E−01	46.536E+00	4.589E+03	1.465E+04
2–9	2P$_0$ 1–2D$_e$ 3	2–6	2.45E+01	6.4603E−01	47.845E+00	1.145E+05	1.069E+05
3–12	2S$_e$ 2–4P$_O$ 5	2–6	2.96E+01	8.545E+00	48.545E+00	1.373E+00	5.267E−02
6–12	4P$_e$ 3–4P$_0$ 5	2–6	6.56E+02	47.033E+00	48.545E+00	1.003E−05	5.267E−02
8–12	2P$_e$ 3–4P$_0$ 5	2–6	8.06E+02	47.388E+00	48.545E+00	1.341E−07	2.150E−02
4–13	4P$_e$ 3–4P$_0$ 3	6–2	4.87E+02	46.536E+00	48.741E+00	4.275E−04	1.064E−01
9–13	2D$_e$ 3–4P$_0$ 3	6–2	1.13E+03	47.84E+00	48.741E+00	2.248E−06	7.273E−03
3–14	4P$_o$ 5–4D$_0$ 3	6–2	2.95E+01	8.545E+00	48.806E+00	1.592E+01	0.00E+00

Table 4 continued

$i\text{–}j$	$T_iC_i\text{–}T_jC_j$	$g_i\text{–}g_j$	λ (Å)	E_i (Ry)	E_j (Ry)	A_{ji}	
						E3	M2
5–14	$2S_e$ 2–$4D_0$ 5	2–8	5.18E+02	46.770E+00	48.806E+00	1.489E−03	6.172E−02
6–14	$4P_e$ 3–$4D_0$ 5	4–8	5.77E+02	47.033E+00	48.806E+00	7.528E−04	0.00E+00
7–14	$4P_e$ 3–$4D_0$ 5	2–8	6.03E+02	47.148E+00	48.806E+00	2.754E−04	3.192E−01
8–14	$2P_e$ 3–$4D_0$ 5	4–8	6.90E+02	47.388E+00	48.806E+00	7.337E−07	0.00E+00
10–14	$2P_e$ 3–$4D_0$ 5	2–8	1.06E+03	47.870E+00	48.806E+00	1.756E−07	6.212E−03
3–15	$2D_e$ 3–$4D_0$ 5	4–8	2.94E+01	8.545E+00	48.841E+00	2.041E+01	3.051E+02
6–15	2 S_e 3–$4D_0$ 5	2–6	5.70E+02	47.033E+00	48.841E+00	5.33E−05	5.005E−02
8–15	$2S_e$ 2–$4D_0$ 5	2–6	6.80E+02	47.388E+00	48.841E+00	1.826E−04	3.216E−02
12–16	$4P_e$ 3–$4D_0$ 5	2–8	3.65E+03	48.545E+00	48.919E+00	2.233E−10	4.275E−05
14–16	$2P_e$ 3–$4D_0$ 5	2–6	1.52E+04	48.806E+00	48.919E+00	9.955E−13	0.00E+00
15–16	2 S_e 3–$4D_0$ 5	2–6	2.28E+04	48.841E+00	48.919E+00	6.578E−14	1.039E−08
(d)							
2–4	$2P_0$ 1–$4P_e$ 3	2–6	16.19308	9.349E−01	5.721E+01	1.577E+04	2.665E+04
2–9	$2P_0$ 1–$2D_e$ 3	2–6	15.86879	9.349E−01	5.836E+01	2.605E+05	2.556E+05
3–12	$2S_e$ 2–$4P_O$ 5	2–6	18.26699	9.702E+00	5.959E+01	6.232E+00	2.96E+02
6–12	$4P_e$ 3–$4P_0$ 5	2–6	532.9047	5.788E+01	5.959E+01	1.772E−05	1.055E−01
8–12	$2P_e$ 3–$4P_0$ 5	2–6	729.0137	5.834E+01	5.959E+01	3.848E−07	2.364E−02
4–13	$4P_e$ 3–$4P_0$ 5	6–2	346.4894	5.721E+01	5.984E+01	8.672E−04	9.197E−02
9–13	$2D_e$ 3–$4P_0$ 5	6–2	615.721	5.836E+01	5.984E+01	4.131E−06	1.475E−02
3–14	$2S_e$ 2–$4D_0$ 5	2–8	18.15418	9.704E+00	5.990E+01	3.615E+01	0.00E +00
5–14	$2P_e$ 3–$4D_0$ 5	4–8	379.6946	5.750E+01	5.990E+01	2.218E−03	1.612E−01
6–14	$4P_e$ 3–$4D_0$ 5	2–8	451.1223	5.788E+01	5.990E+01	9.44E−04	0.00E+00
7–14	$4P_e$ 3–$4D_0$ 5	4–8	497.9602	5.807E+01	5.990E+01	3.629E−04	3.861E−01
8–14	$2P_e$ 3–$4D_0$ 5	2–8	584.1456	5.834E+01	5.990E+01	5.964E−06	0.00E+00
10–14	$2D_e$ 3–$4D_0$ 5	4–8	884.7253	5.887E+01	5.990E+01	2.938E−07	1.185E−02
3–15	$2S_e$ 2–$2D_0$ 5	2–6	18.14695	9.704E+00	5.992E+01	4.853E+01	6.867E+02
6–15	$4P_e$ 3–$2D_0$ 5	2–6	446.6996	5.788E+01	5.992E+01	8.779E−05	5.929E−02
8–15	$2P_e$ 3–$2D_0$ 5	2–6	576.7513	5.834E+01	5.992E+01	1.722E−04	2.218E−02
(e)							
2–4	$2P_0$ 1–$4P_e$ 3	2–6	16.35733	1.311E+01	6.882E+01	4.276E+04	4.07E+04
2–9	$2P_0$ 1–$2D_e$ 3	2–6	15.79319	1.311E+01	7.081E+01	5.498E+05	5.626E+05
3–12	$2S_e$ 2–$4P_O$ 5	2–6	15.11222	1.103E+01	7.133E+01	2.677E+01	1.022 +00
6–12	$4P_e$ 3–$4P_0$ 5	2–6	548.9561	6.967E+01	7.133E+01	1.502E−05	1.067E−01
8–12	$2P_e$ 3–$4P_0$ 5	2–6	836.0249	7.024E+01	7.133E+01	3.584E−07	8.359E−03
4–13	$4P_e$ 3–$4P_0$ 5	6–2	320.8687	6.882E+01	7.166E+01	8.946E−04	3.191E−02
9–13	$2D_e$ 3–$4P_0$ 5	6–2	1072.079	7.081E+01	7.166E+01	1.090E−06	6.906E−03
3–14	$2S_e$ 2–$4D_0$ 5	6–2	15.01511	1.103E+01	7.172E+01	8.21E+01	1.788E+03
6–14	$4P_e$ 3–$4D_0$ 5	4–8	444.5205	6.967E+01	7.172E+01	7.713E−05	2.398E−02
8–14	$2P_e$ 3–$4D_0$ 5	4–8	615.721	7.024E+01	7.172E+01	5.856E−05	4.279E−03
3–15	$2S_e$ 2–$4D_0$ 5	2–8	15.01016	1.103E+01	7.174E+01	7.196E+01	0.00E+00
5–15	$2D_e$ 3–$4D_0$ 5	4–8	346.4894	6.911E+01	7.174E+01	2.038E−03	2.709E−01
6–15	2 S_e 3–$4D_0$ 5	2–6	440.2257	6.967E+01	7.174E+01	6.082E−04	0.00
7–15	$2S_e$ 2–$4D_0$ 5	2–6	517.7654	6.998E+01	7.174E+01	1.953E−04	2.386E−01
8–15	$4P_e$ 3–$4D_0$ 5	2–8	312.0778	6.882E+01	7.174E+01	8.046E−06	0.00
10–15	$2P_e$ 3–$4D_0$ 5	2–6	1035.531	7.086E+01	7.174E+01	8.748E−08	6.163E−03
4–16	2 S_e 3–$4D_0$ 5	2–6	262.613	6.882E+01	7.229E+01	5.461E−03	7.741E−01
9–16	$2D_e$ 3–$4D_0$ 5	6–2	615.721	7.081E+01	7.229E+01	2.982E−05	2.414E−04

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