Energy levels, oscillator strengths, transition probabilities and lifetimes of the O-like Cl X ion

Reem Al Salamah, Lamia Abu El Maati, Abubaker Siddig, Nabil Ben Nessib, Milan S Dimitrijević

HAL Id: hal-04613211

https://hal.sorbonne-universite.fr/hal-04613211

Submitted on 15 Jun 2024

Graphical Abstract

Energy levels, oscillator strengths, transition probabilities and lifetimes of the O-like Cl X ion

Reem Al Salamah, Lamia Abu El Maati, Abubaker Siddig, Nabil Ben Nessib, Milan S. Dimitrijević

Energy levels in cm^{-1}

$^3D^o_{1,2,3}$
$^3S^o_{1}$
$^1S_0$
$^3P^o_{1,2,3}$
$^1S_0$
$^1D_2$
$^3P_0$
$^3P_1$
$^3P_2$

1000000
100000
10000
0

$2s^2 2p^4$ $2s2p^5$ $2p^6$ $2s^2 2p^3 3s$
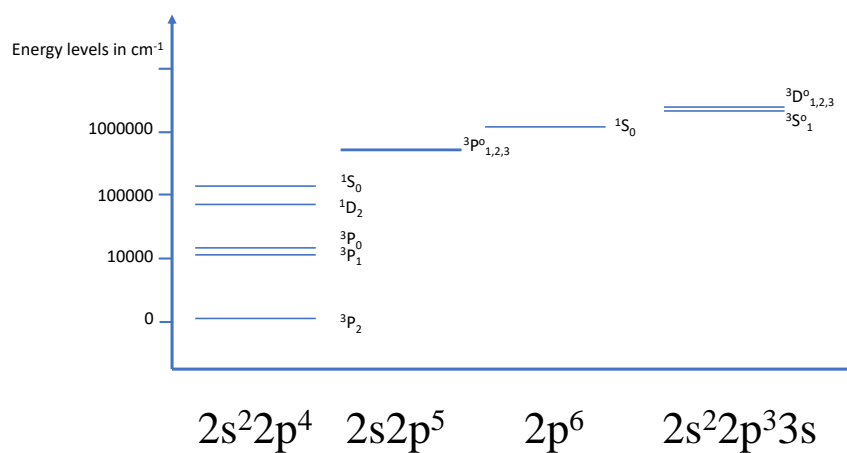
Highlights

Energy levels, oscillator strengths, transition probabilities and lifetimes of the O-like Cl X ion

Reem Al Salamah, Lamia Abu El Maati, Abubaker Siddig, Nabil Ben Nessib, Milan S. Dimitrijević

- Energy levels and lifetimes for the lowest fine-structure levels of Cl X ion are calculated.

- Comparison of the calculated energy levels and lifetimes with experimental and other theoretical calculation values.

- Calculations of the oscillator strengths and transition probabilities of the Cl X ion.

- Comparison of the calculated transition parameters with experimental and other calculated values.

Energy levels, oscillator strengths, transition probabilities and lifetimes of the O-like Cl X ion

Reem Al Salamah[a], Lamia Abu El Maati[b], Abubaker Siddig[a], Nabil Ben Nessib[a], Milan S. Dimitrijević[c,d]

[a]*Department of Physics and Astronomy, College of Sciences, King Saud University, Riyadh, 11451, Riyadh, Saudi Arabia*
[b]*Department of Physics, Faculty of Science, Benha University, Benha, 13513, Benha, Egypt*
[c]*Astronomical Observatory, Volgina 7, Belgrade 38, 11060, Belgrade, Serbia*
[d]*LERMA, Observatoire de Paris, University PSL, CNRS, Sorbonne University, 5 Place Jules Janssen, Meudon, 92190, Meudon, France*

Abstract

Energy levels, lifetimes, oscillator strengths and transition probabilities for the multicharged oxygen like Cl X ion have been calculated with the configuration expansion: $2s^2 2p^4$, $2p^6$, $2s^2 2p^3 3p$, $2s2p^5$, $2s^2 2p^3 3s$, $2s^2 2p^3 4s$, $2s^2 2p^3 3d$, $2s^2 2p^3 4d$, $2s2p^4 3s$ and $2s2p^4 4s$. We used two methods in the calculations: the Hartree-Fock pseudo-relativistic approach and the Thomas-Fermi-Dirac-Amaldi potential approach using the Cowan and the AUTOSTRUCTURE atomic structure codes respectively. Results have been compared with available experimental data from the National Institute of Standards and Technology Atomic Spectra Database (NIST-ASD) and with results from other available calculations.

There is a great lack of atomic structure data of Cl X and obtained new data will be important for physics applications and astrophysical modeling.

Keywords: energy levels, oscillator strengths, transition probabilities, lifetimes
PACS: 32.30.-r, 32.70.Cs

Email address: `mdimitrijevic@aob.rs` (Milan S. Dimitrijević)

1. Introduction

Oxygen-like ions are important in plasma laboratories and astrophysical studies, but there is a luck of sufficiently comprehensive theoretical studies of the spectral characteristics of these ions. O-like ions of low and medium Z exist in various high-temperature plasma sources, so their spectrum is fundamental in high-temperature plasma research [1, 2].

In [1] *ab initio* wavelengths and oscillator strengths of 5 configurations for the oxygen-like chlorine Cl X ion have been calculated.

In [3] energy spectra of the ground and four excited configurations ($2s2p^5$ and $2s^2 2p^3 3\ell$) and the radiative lifetimes of the excited levels are investigated. The calculations of the five O-like ions Mg V, Si VII, Cl X, Ca XIII, and Cr XVII are taken as examples, they are performed based on the transformed radial orbitals.

Forbidden transition energies and magnetic dipole transition probabilities of $2s^2 2p^4(^3P_1 - ^3P_2)$ and $2s^2 2p^4(^3P_0 - ^3P_1)$ of O-like isoelectronic sequences (Z from 10 to 32) are calculated by Yong et al. [4] with polarization potential correction method.

Rynkun et al. [5] calculated energy levels and E1, M1, E2, and M2 transition rates for states of the $2s^2 2p^4$, $2s2p^5$, and $2p^6$ configurations in O-like ions between F II and Kr XXIX using the multi-configuration Dirac-Hartree-Fock (MCDHF) method.

In precedent works, we calculated atomic structure of the first elements of the carbon-like sequence: In the first work concerning the atomic structure in the C-like elements [6], we calculated excitation energies and oscillator strengths for the $2s^2 2p^2$, $2s2p^3$, $2s^2 2p3s$, $2s^2 2p3p$, $2s^2 2p3d$, $2s^2 2p4s$, $2s^2 2p4p$, and $2s^2 2p5s$ configurations in C-like elements from C I to Ne V, using the three different codes: Cowan (CW) [7, 8], SUPERSTRUCTURE (SS) [9], and AUTOSTRUCTURE (AS) [10]. The first code uses the Hartree-Fock pseudo-relativistic (HFR) approach and the two latest codes use the Thomas-Fermi-Dirac-Amaldi (TFDA) potential method.

We extended this purely *ab initio* HFR and TFDA calculations to semi-empirical data in the C-like sequence from Na VI to Ar XIII [11]. We also added the transition probabilities calculation of these C-like ions.

In [12], we calculated atomic structure and transition parameters of the Ca XIV C-like ion using the suite of atomic structure codes of GRASP2018 [13]. The configuration expansion of the basis set used consists of 4 even parity configurations: $2s^2 2p^2$ and $2s^2 2p$ np (n = 3 - 5) and 5 odd parity

2

configurations: 2s 2p^3, 2s^2 2p ns (n = 3 - 5) and 2s^2 2p 3d. Energy levels and oscillator strengths obtained with the GRASP2018 code have been compared with data from NIST-ASD [14] and other theoretical methods.

We also studied the atomic structure and transition parameters of the C-like ion V XVIII using both the TFDA and MCDHF approaches [15].

In the present work, the HFR and TFDA approaches are used to calculate energy levels, E1 radiative transition parameters of the 10 configurations: 2s^{2}2p^4, 2p^6, 2s^{2}2p^{3}3p, 2s2p^5, 2s^{2}2p^{3}3s, 2s^{2}2p^{3}4s, 2s^{2}2p^{3}3d, 2s^{2}2p^{3}4d, 2s2p^{4}3s and 2s2p^{4}4s in Cl X ion. In section 2, we present the theoretical approaches used in this work, and in section 3, we present our results and compare them to the available data in the literature. We finish the paper with the conclusions in section 4 where we show the importance of this work in physics and astrophysics.

2. Theoretical Approaches

Calculations are made with the pseudo-relativistic Hartree-Fock (HFR) and the Thomas-Fermi-Dirac-Amaldi (TFDA) potential approaches implemented in Cowan's and AUTOSTRUCTURE's atomic structure codes respectively.

2.1. Hartree-Fock pseudo-relativistic (HFR) approach

In this approach, we approximate the wave functions by an anti-symmetric combination of hydrogenic ones:

$$\psi(1,2,3,........N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_\alpha(1) & \psi_\alpha(2) & .... & \psi_\alpha(N) \\ \psi_\beta(1) & \psi_\beta(2) & & \psi_\beta(N) \\ .... & & & \\ \psi_\nu(1) & \psi_\nu(2) & .... & \psi_\nu(N) \end{vmatrix} \quad (1)$$

where, 1, 2, 3, ... N, refer to the set of coordinates and the projection of the spin of each electron, and $\alpha, \beta, ...\nu$ are sets of quantum numbers.

This theoretical method is used in the Cowan (CW) atomic structure code [7, 8]. The first three programs of the CW code are RCN, RCN2, and RCG, they are needed for *ab initio* calculations. The fourth program (RCE) is for semi-empirical atomic structure parameter calculations, it uses the Least-Square Fitting (LSF) of energy levels.

2.2. Thomas-Fermi-Dirac-Amaldi (TFDA) potential method

In this approach, we use the Thomas-Fermi-Dirac-Amaldi (TFDA) potential as a simplified potential V instead of the simplified wave function ψ used in the HFR method.

$$V(r) = \frac{Z_{eff}(\lambda_{n\ell}, r)}{r} = -\frac{Z}{r}\varphi(x) \tag{2}$$

where

$$\varphi(x) = e^{-\frac{Zr}{2}} + \lambda_{n\ell}\left(1 - e^{-\frac{Zr}{2}}\right), x = \frac{r}{\mu}$$

and

$$\mu = \frac{1}{4}\left(\frac{N}{N-1}\right)^{2/3}\left(\frac{9\pi^2}{2Z}\right)^{1/3} \approx 0.8853\left(\frac{N}{N-1}\right)^{2/3}(Z)^{-1/3}$$

$\lambda_{n\ell}$ are the orbital scaling parameters. They are determined variationally by minimizing the sum of energies of all target terms. Z is the atomic number and N number of electrons in the studied ion. Z_{eff} is the effective charge function depending on $\lambda_{n\ell}$ and r.

This second theoretical method is used by AUTOSTRUCTURE (AS) atomic structure code [10, 16] which is an extension of the SS code. The original version in 1974 of SS is by Eissner *et al* [9]. An updated version of the SS atomic structure code ([17]) with some relativistic corrections is introduced and orbital scaling parameters λ are dependent on n and ℓ unlike the original SS version of 1974 [9]. In this original version, scaling parameters depend only on ℓ (λ_ℓ). The AS code [10, 16] is an extension of the SS code incorporating various improvements and new capabilities like two-body non-fine-structure operators of the Breit-Pauli Hamiltonian and polarization model potentials [18].

Energy levels in SS and AS atomic structure codes can be improved by means of semi-empirical corrections to the term energies [19] to have data adjusted with experimental values. Term Energy Correction (TEC) and Level Energy Correction (LEC) are the differences between the measured and calculated term and level energy respectively. These TEC or LEC parameters are introduced to make a semi-empirical calculation of energies.

3. Results and discussions

In the present work, both calculations with the CW (HFR method) and AS (TFDA method) atomic structure codes, were performed for the states

belonging to the six even configurations: $2s^22p^4$, $2p^6$, $2s^22p^33p$, $2s^22p^34p$, $2s2p^43s$ and $2s2p^44s$ and the four odd configurations: $2s2p^5$, $2s^22p^33s$, $2s^22p^34s$ and $2s^22p^33d$ in the O-like Cl X ion.

As a starting point, *ab initio* calculations were performed using both HFR and TFDA methods.

For the semi-empirical calculations with the HFR method, a parametric Least-Squares-Fitted (LSF) was performed to minimize the differences between the theoretical and observed energy level values from NIST-ASD values [14]. We present the LSF parameters used in the Cowan calculations in Table 1.

For the semi-empirical calculations with the TFDA potential method, we used the LEC as the difference between the NIST-ASD energy level values and our *ab initio* obtained values. We present the Thomas-Fermi-Dirac-Amaldi potential scaling parameters used in the AUTOSTRUCTURE calculations in Table 2.

5

Table 1: Parameters of the Least-Squares Fit (LSF) of Cl X energy levels with Cowans code.

Configuration		parameter	LSF	Uncert.	Group	HF	LSF/HF
$2s^2 2p^4$		E_{av}	35611.4	31		34775.7	1.0240
		$F^2(2p,2p)$	243259.5	257		252910	0.9618
		$\alpha(2p)$	0	fixed		0	
		$\zeta(2p)$	10020.9	52		9737.5	1.0291
$2p^6$		E_{av}	1119118.3	159		1148828.1	0.9741
$2s^2 2p^4$	$2p^6$	$R_D^1(2s,2s;2p,2p)$	226567.4	968		291492.1	0.7773
$2s^2 2p^4$	$2s^2 2p^3\ 3p$	$R_D^0(2p,2p;2p,3p)$	9758.4	fixed		10381.3	0.94
		$R_D^2(2p,2p;2p,3p)$	44654.9	fixed		47505.2	0.94
$2s\ 2p^5$		E_{av}	548123.2	24077		548123.2	1
		$\zeta(2p)$	9586.7	461	1	9586.7	1
		$G^1(2s,2p)$	274087.4	6394	2	291582.34	0.94
$2s^2 2p^3\ 3s$		E_{av}	2206069.2	392		2206069.2	1
		$F^2(2p,2p)$	245208.7	fixed		260860.319	0.94
		$\alpha(2p)$	0	fixed		0	
		$\zeta(2p)$	10354	498	1	10354	1
		$G^1(2p,3s)$	21429.6	500	2	22797.447	0.94
$2s^2 2p^3\ 3d$		E_{av}	2490507.5	fixed		2490507.5	1
		$F^2(2p,2p)$	245029.5	fixed		260669.681	0.94
		$\alpha(2p)$	0	fixed		0	
		$\zeta(2p)$	10371.6	fixed		10371.6	1
		$\zeta(3d)$	202.2	fixed		202.2	1
		$F^1(2p,3d)$	0	fixed		0	
		$F^2(2p,3d)$	66015.3	fixed		70229.043	0.94
		$G^1(2p,3d)$	56987.1	fixed		60624.574	0.94
		$G^2(2p,3d)$	0	fixed		0	
		$G^3(2p,3d)$	32756.9	fixed		34847.766	0.94
$2s\ 2p^5$	$2s^2 2p^3\ 3s$	$R_D^1(2p,2p;2s,3s)$	47440.2	525387		50468.3	0.94
$2s\ 2p^5$	$2s^2 2p^3\ 3d$	$R_D^1(2p,2p;2s,3d)$	-119799.2	fixed		-127446	0.94
$2s^2 2p^3\ 3s$	$2s^2 2p^3\ 3d$	$R_D^2(2p,3s;2p,3d)$	18093.2	fixed		19248.1	0.94
		$R_E^1(2p,3s;2p,3d)$	-11915.6	fixed		-12676.2	0.94

Table 2: Thomas-Fermi-Dirac-Amaldi potential scaling parameters used in the AUTOSTRUCTURE calculations

1s	2s	2p	3s	3p	3d
1.45964	1.24795	1.18724	1.20167	1.12104	1.17177

3.1. Energy levels

The energy levels are presented in Table 3. We present the energy levels calculated with the HFR and TFDA approaches using the atomic structure

codes CW and AS respectively.

Table 3: Energy levels. E(NIST) are the values from the NIST database. E(CW) and E(AS) were our calculations using respectively the Cowan (CW) and AUTOSTRUCTURE (AS) codes. E(MCHF) are the values calculated by Froese Fischer and Tachiev [20, 21] using the MCHF method. E(MCDHF) are the values calculated by Rynkun et al. [5] using the MCDHF method. All energies are in cm^{-1}.

K	Configuration	Term	J	E(NIST)	E(CW)	E(AS)	E(MCHF)	E(MCDHF)
1	$2s^22p^4$	^{3}P	2	0	0	0	0	0
2	$2s^22p^4$	^{3}P	1	10847	10809	10893	10924	10848
3	$2s^22p^4$	^{3}P	0	14127	14161	14186	14095	14128
4	$2s^22p^4$	^{1}D	2	64782	64782	64880	65297	64913
5	$2s^22p^4$	^{1}S	0	135206	135206	133644	135168	135507
6	$2s2p^5$	^{3}P^o	2	486894	486829	486965	488539	487130
7	$2s2p^5$	^{3}P^o	1	496276	496369	496367	497979	496517
8	$2s2p^5$	^{3}P^o	0	501554	501526	501626	503294	501819
9	$2s2p^5$	^{1}P^o	1		682207	701315	675277	673161
10	$2p^6$	^{1}S	0	1136464	1136464	1138154	1140126	1137322
11	$2s^22p^3(^4S^o)3s$	^{5}S^o	2		2105388	2100238	2105093	
12	$2s^22p^3(^4S^o)3s$	^{3}S^o	1	2134700	2134702	2134720	2135217	
13	$2s^22p^3(^4S^o)3s$	^{3}D^o	1	2200800	2200827	2200831	2202069	
14	$2s^22p^3(^4S^o)3s$	^{3}D^o	2	2201200	2201324	2201227	2202414	
15	$2s^22p^3(^4S^o)3s$	^{3}D^o	3	2202900	2202753	2202942	2203704	
16	$2s^22p^3(^4S^o)3s$	^{1}D^o	2	2216400	2216394	2216434	2217752	
17	$2s^22p^3(^4S^o)3p$	^{5}P	1		2227644	2219903	2228627	
18	$2s^22p^3(^4S^o)3p$	^{5}P	2		2228525	2220694	2229526	
19	$2s^22p^3(^4S^o)3p$	^{5}P	3		2230145	2222243	2231245	
20	$2s^22p^3(^4S^o)3p$	^{3}P	1		2257031	2251080	2257206	
21	$2s^22p^3(^4S^o)3p$	^{3}P	2		2257629	2251598	2257843	
22	$2s^22p^3(^4S^o)3p$	^{3}P	0		2258050	2252187	2258360	
23	$2s^22p^3(^4S^o)3s$	^{3}P^o	0		2262325	2263293	2251135	
24	$2s^22p^3(^4S^o)3s$	^{3}P^o	1		2263247	2264046	2252034	
25	$2s^22p^3(^4S^o)3s$	^{3}P^o	2		2265529	2265942	2254485	
26	$2s^22p^3(^4S^o)3s$	^{1}P^o	1		2278893	2280082	2268214	

Table 3 – continued

K	Configuration	Term	J	E(NIST)	E(CW)	E(AS)	E(MCHF)	E(MCDHF)
27	2s^{2}2p^3(^{2}D^o)3p	^{1}P	1		2309103	2306340	2311264	
28	2s^{2}2p^3(^{2}D^o)3p	^{3}D	2		2315208	2312391	2318105	
29	2s^{2}2p^3(^{2}D^o)3p	^{3}D	1		2317231	2314233	2320067	
30	2s^{2}2p^3(^{2}D^o)3p	^{3}D	3		2317734	2314509	2320611	
31	2s^{2}2p^3(^{2}D^o)3p	^{3}F	2		2324346	2322833	2327292	
32	2s^{2}2p^3(^{2}D^o)3p	^{3}F	3		2326180	2324279	2329100	
33	2s^{2}2p^3(^{2}D^o)3p	^{3}F	4		2328195	2325831	2330847	
34	2s^{2}2p^3(^{2}D^o)3p	^{1}F	3		2331884	2330297	2334250	
35	2s^{2}2p^3(^{2}D^o)3p	^{3}P	1		2362071	2361614	2398110	
36	2s^{2}2p^3(^{2}D^o)3p	^{3}P	0		2362003	2361837	2364307	
37	2s^{2}2p^3(^{2}D^o)3p	^{3}P	2		2365615	2364341	2366824	
38	2s^{2}2p^3(^{2}P^o)3p	^{3}S	1		2379192	2378852	2360895	
39	2s^{2}2p^3(^{4}S^o)3d	^{5}D^o	0		2386574	2379606	2386278	
40	2s^{2}2p^3(^{4}S^o)3d	^{5}D^o	1		2386623	2379611	2386290	
41	2s^{2}2p^3(^{4}S^o)3d	^{5}D^o	2		2386713	2379625	2386304	
42	2s^{2}2p^3(^{4}S^o)3d	^{5}D^o	3		2386843	2379665	2386321	
43	2s^{2}2p^3(^{4}S^o)3d	^{5}D^o	4		2387044	2379799	2386399	
44	2s^{2}2p^3(^{2}D^o)3p	^{1}D	2		2381053	2381673	2382663	
45	2s^{2}2p^3(^{2}P^o)3p	^{3}D	1		2384360	2385240	2376382	
46	2s^{2}2p^3(^{2}P^o)3p	^{3}D	3		2387967	2388289	2379776	
47	2s^{2}2p^3(^{2}P^o)3p	^{3}D	2		2387542	2388293	2376491	
48	2s^{2}2p^3(^{2}P^o)3p	^{1}P	1		2394168	2395073	2387580	
49	2s^{2}2p^3(^{2}P^o)3p	^{3}P	2		2405897	2406538	2397435	
50	2s^{2}2p^3(^{2}P^o)3p	^{3}P	1		2407296	2407774		
51	2s^{2}2p^3(^{2}P^o)3p	^{3}P	0		2407918	2408309	2398554	
52	2s^{2}2p^3(^{4}S^o)3d	^{3}D^o	2		2418435	2413117	2416149	
53	2s^{2}2p^3(^{4}S^o)3d	^{3}D^o	1		2418834	2413594	2416685	
54	2s^{2}2p^3(^{4}S^o)3d	^{3}D^o	3		2419607	2414161	2417290	
55	2s^{2}2p^3(^{2}P^o)3p	^{1}D	2		2429112	2431378	2419775	
56	2s^{2}2p^3(^{2}D^o)3d	^{3}F^o	2		2471606	2469936	2471963	
57	2s^{2}2p^3(^{2}D^o)3d	^{3}F^o	3		2473613	2471613	2474096	
58	2s^{2}2p^3(^{2}D^o)3d	^{1}S^o	0		2474998	2472921	2475337	
59	2s^{2}2p^3(^{2}D^o)3d	^{3}F^o	4		2475984	2473637	2476619	
60	2s^{2}2p^3(^{2}D^o)3d	^{3}G^o	3		2480134	2478932	2483765	
61	2s^{2}2p^3(^{2}D^o)3d	^{3}G^o	4		2480995	2479498	2484455	
62	2s^{2}2p^3(^{2}D^o)3d	^{3}G^o	5		2481991	2479988	2485166	

Table 3 – continued

K	Configuration	Term	J	E(NIST)	E(CW)	E(AS)	E(MCHF)	E(MCDHF)
63	$2s^2 2p^3(^2D^o)3d$	$^1G^o$	4		2485077	2483580	2487776	
64	$2s^2 2p^3(^2P^o)3p$	^1S	0		2478704	2483845	2465895	
65	$2s^2 2p^3(^2D^o)3d$	$^3D^o$	1		2491169	2490555	2497212	
66	$2s^2 2p^3(^2D^o)3d$	$^3D^o$	2		2495377	2494526	2496179	
67	$2s^2 2p^3(^2D^o)3d$	$^1P^o$	1		2496590	2495447	2491670	
68	$2s^2 2p^3(^2D^o)3d$	$^3D^o$	3		2496682	2495570	2496962	
69	$2s^2 2p^3(^2D^o)3d$	$^3P^o$	2		2505163	2504667	2505143	
70	$2s^2 2p^3(^2D^o)3d$	$^3P^o$	0		2506937	2506730	2508941	
71	$2s^2 2p^3(^2D^o)3d$	$^3P^o$	1		2507081	2506773	2508773	
72	$2s^2 2p^3(^2D^o)3d$	$^1D^o$	2		2508207	2507836	2506179	
73	$2s^2 2p^3(^2D^o)3d$	$^3S^o$	1		2512761	2512755	2515669	
74	$2s2p^4(^4P)3s$	^5P	3		2527529	2515472	2529026	
75	$2s2p^4(^4P)3s$	^5P	2		2535061	2523470	2536994	
76	$2s^2 2p^3(^2D^o)3d$	$^1F^o$	3		2527418	2528159	2526410	
77	$2s2p^4(^4P)3s$	^5P	1		2539825	2528337	2541784	
78	$2s^2 2p^3(^2P^o)3d$	$^3F^o$	4		2542922	2543770	2534602	
79	$2s^2 2p^3(^2P^o)3d$	$^3F^o$	2		2542863	2544203	2535437	
80	$2s^2 2p^3(^2P^o)3d$	$^3F^o$	3		2543185	2544375	2535542	
81	$2s^2 2p^3(^2P^o)3d$	$^3P^o$	0		2546439	2547638	2536000	
82	$2s^2 2p^3(^2P^o)3d$	$^3P^o$	1		2547345	2548504	2537877	
83	$2s^2 2p^3(^2P^o)3d$	$^3P^o$	2		2548308	2549488	2539640	
84	$2s^2 2p^3(^2P^o)3d$	$^3D^o$	2		2556745	2558798	2547396	
85	$2s^2 2p^3(^2P^o)3d$	$^3D^o$	3		2558811	2560549	2550010	
86	$2s^2 2p^3(^2P^o)3d$	$^3D^o$	1		2559975	2562014	2550059	
87	$2s2p^4(^4P)3s$	^3P	2		2574276	2565202		
88	$2s^2 2p^3(^2P^o)3d$	$^1D^o$	2		2565262	2567313	2558292	
89	$2s2p^4(^4P)3s$	^3P	1		2582621	2574005		
90	$2s^2 2p^3(^2P^o)3d$	$^1F^o$	3		2572738	2575523	2561852	
91	$2s2p^4(^4P)3s$	^3P	0		2586390	2577836		
92	$2s^2 2p^3(^2P^o)3d$	$^1P^o$	1		2600955	2605045	2589190	
93	$2s2p^4(^2D)3s$	^3D	1		2692983	2690708		
94	$2s2p^4(^2D)3s$	^3D	2		2693261	2690886		
95	$2s2p^4(^2D)3s$	^3D	3		2693650	2691125		
96	$2s2p^4(^2D)3s$	^1D	2		2723625	2722089		
97	$2s2p^4(^2S)3s$	^3S	1		2779688	2781988		
98	$2s2p^4(^2S)3s$	^1S	0		2809354	2812977		

Table 3 – continued

K	Configuration	Term	J	E(NIST)	E(CW)	E(AS)	E(MCHF)	E(MCDHF)
99	$2s2p^4(^2P)3s$	^3P	2		2822403	2825738		
100	$2s2p^4(^2P)3s$	^3P	1		2827045	2830674		
101	$2s2p^4(^2P)3s$	^3P	0		2835513	2839140		
102	$2s2p^4(^2P)3s$	^1P	1		2839335	2843773		
103	$2s^22p^3(^4S^o)4s$	$^5S^o$	2		2899579	2848884		
104	$2s^22p^3(^4S^o)4s$	$^3S^o$	1		2904254	2859027		
105	$2s^22p^3(^4S^o)4p$	^5P	1		2907082	2897042		
106	$2s^22p^3(^4S^o)4p$	^5P	2		2907448	2897372		
107	$2s^22p^3(^4S^o)4p$	^5P	3		2908088	2897984		
108	$2s^22p^3(^4S^o)4p$	^3P	1		2921841	2913206		
109	$2s^22p^3(^4S^o)4p$	^3P	2		2922064	2913310		
110	$2s^22p^3(^4S^o)4p$	^3P	0		2922263	2913713		
111	$2s^22p^3(^2D^o)4s$	$^3D^o$	1		2948028	2943869		
112	$2s^22p^3(^2D^o)4s$	$^3D^o$	2		2948564	2944228		
113	$2s^22p^3(^2D^o)4s$	$^3D^o$	3		2950039	2945141		
114	$2s^22p^3(^2D^o)4s$	$^1D^o$	2		2953068	2949709		
115	$2s^22p^3(^2D^o)4p$	^3D	1		2994101	2989369		
116	$2s^22p^3(^2D^o)4p$	^3D	2		2995810	2990733		
117	$2s^22p^3(^2D^o)4p$	^3D	3		2997890	2991827		
118	$2s^22p^3(^2D^o)4p$	^3F	2		2996710	2992085		
119	$2s^22p^3(^2D^o)4p$	^3F	3		2997265	2993038		
120	$2s^22p^3(^2D^o)4p$	^1P	1		2998763	2993682		
121	$2s^22p^3(^2D^o)4p$	^3F	4		2999364	2993971		
122	$2s^22p^3(^2D^o)4p$	^1F	3		3000172	2995125		
123	$2s^22p^3(^2D^o)4p$	^3P	0		3009506	3005847		
124	$2s^22p^3(^2D^o)4p$	^3P	1		3010255	3006305		
125	$2s^22p^3(^2D^o)4p$	^3P	2		3011429	3006933		
126	$2s^22p^3(^2P^o)4s$	$^3P^o$	0		3010020	3007340		
127	$2s^22p^3(^2P^o)4s$	$^3P^o$	1		3011675	3007944		
128	$2s^22p^3(^2P^o)4s$	$^3P^o$	2		3012134	3009849		
129	$2s^22p^3(^2P^o)4s$	$^1P^o$	1		3016082	3014186		
130	$2s^22p^3(^2D^o)4p$	^1D	2		3022818	3019679		
131	$2s^22p^3(^2P^o)4p$	^3D	1		3057173	3054865		
132	$2s^22p^3(^2P^o)4p$	^3S	1		3058202	3055512		
133	$2s^22p^3(^2P^o)4p$	^3D	2		3058873	3056393		
134	$2s^22p^3(^2P^o)4p$	^3D	3		3060669	3057874		

Table 3 – continued

K	Configuration	Term	J	E(NIST)	E(CW)	E(AS)	E(MCHF)	E(MCDHF)
135	$2s^22p^3(^2P^o)4p$	^1P	1		3061818	3059320		
136	$2s^22p^3(^2P^o)4p$	^3P	0		3066009	3063861		
137	$2s^22p^3(^2P^o)4p$	^3P	1		3066625	3064315		
138	$2s^22p^3(^2P^o)4p$	^3P	2		3067009	3064628		
139	$2s^22p^3(^2P^o)4p$	^1D	2		3070883	3069112		
140	$2s^22p^3(^2P^o)4p$	^1S	0		3094998	3095420		
141	$2s2p^4(^4P)4s$	^5P	3		3274537	3258696		
142	$2s2p^4(^4P)4s$	^5P	2		3281564	3266148		
143	$2s2p^4(^4P)4s$	^5P	1		3286865	3271554		
144	$2s2p^4(^4P)4s$	^3P	2		3290857	3276239		
145	$2s2p^4(^4P)4s$	^3P	1		3298873	3284660		
146	$2s2p^4(^4P)4s$	^3P	0		3302463	3288304		
147	$2s2p^4(^2D)4s$	^3D	1		3433991	3427338		
148	$2s2p^4(^2D)4s$	^3D	2		3434229	3427486		
149	$2s2p^4(^2D)4s$	^3D	3		3434599	3427710		
150	$2s2p^4(^2D)4s$	^1D	2		3444907	3438721		
151	$2s2p^4(^2S)4s$	^3S	1		3521289	3519096		
152	$2s2p^4(^2S)4s$	^1S	0		3531630	3530161		
153	$2s2p^4(^2P)4s$	^3P	2		3560411	3559859		
154	$2s2p^4(^2P)4s$	^1P	1		3562524	3562194		
155	$2s2p^4(^2P)4s$	^3P	0		3572220	3571951		
156	$2s2p^4(^2P)4s$	^3P	1		3573096	3573028		

For Cl X, there are only 14 energy levels in the NIST-ASD [14]. Comparing our results of energy levels with these energy levels in NIST-ASD (see Table 3), we see that the CW and AS calculated values are 0.05% and 0.16% far from the NIST-ASD data respectively. The MCHF calculations by Froese Fischer and Tachiev [20, 21] are 0.24% different from NIST-ASD data. The only 10 common calculated values by Rynkun et al. [5] using MCDHF method differ by 0.07% from NIST-ASD data.

In the fitting process we used the NIST-ASD values as reference data. With the CW atomic structure code and for even parity, all 6 energy levels of the $2s^22p^4$ and $2p^6$ configurations were fitted with a standard deviation of 51 cm^{-1} by 5 free parameters. For odd parity, 8 energy levels of the $2s2p^5$ and $2s^22p^33s$ configurations were fitted with a standard deviation of 131 cm^{-1} by 5 free parameters. With the AS atomic structure code, we used the LEC

method, where in the file SHFTIC we put the difference of the energy levels from NIST and from *ab initio* calculations. A standard deviation of 604 cm^{-1} is obtained between our AS calculations and the NIST-ASD values as references for both parities.

The difference between our both calculations with the HFR and the TFDA is 0.23%. We can see from Table 3 that there is an excellent agreement for calculated energy levels with experimental data from the National Institute of Standards and Technology Atomic Spectra Database (NIST-ASD).

Table 4: Radiative lifetimes. τ(CW) and τ(AS) were our calculations using respectively the Cowan (CW) and AUTOSTRUCTURE (AS) codes. τ(MCHF) are the values calculated by Froese Fischer and Tachiev [20, 21] using the MCHF method.

K	τ(CW)	τ(AS)	τ(MCHF)
6	4.580E-11	4.758E-11	5.338E-11
7	4.430E-11	4.610E-11	5.160E-11
8	4.390E-11	4.558E-11	5.103E-11
9	1.190E-11	1.148E-11	1.441E-11
10	1.540E-11	1.755E-11	1.782E-11
11	2.070E-09	1.822E-09	2.078E-09
12	2.300E-12	2.684E-12	2.423E-12
13	6.900E-12	7.707E-12	7.497E-12
14	6.910E-12	7.857E-12	7.615E-12
15	6.830E-12	7.877E-12	7.544E-12
16	2.820E-12	3.241E-12	3.040E-12
17	7.660E-10	8.177E-10	7.930E-10
18	7.630E-10	8.081E-10	7.909E-10
19	7.420E-10	7.957E-10	7.563E-10
20	3.940E-10	5.034E-10	7.288E-10
21	3.930E-10	4.980E-10	7.183E-10
22	4.090E-10	5.328E-10	7.477E-10
23	6.770E-12	7.763E-12	7.875E-12
24	6.590E-12	7.662E-12	7.650E-12
25	6.380E-12	7.507E-12	7.144E-12
26	2.780E-12	3.266E-12	3.112E-12
27	1.410E-10	1.446E-10	5.752E-10

Table 4 – continued

K	τ(CW)	τ(AS)	τ(MCHF)
28	3.100E-10	3.283E-10	7.281E-10
29	1.620E-10	1.819E-10	5.361E-10
30	2.930E-10	3.109E-10	6.525E-10
31	6.150E-10	6.464E-10	6.347E-10
32	5.820E-10	6.173E-10	6.095E-10
33	6.650E-10	7.022E-10	7.022E-10
34	8.460E-10	8.645E-10	8.190E-10
35	6.210E-11	5.374E-11	2.078E-10
36	6.450E-11	5.439E-11	7.441E-11
37	4.900E-11	4.334E-11	5.991E-11
38	7.500E-11	7.052E-11	7.372E-11
39	2.080E-10	2.045E-10	2.156E-10
40	2.130E-10	2.084E-10	2.216E-10
41	2.420E-10	2.358E-10	2.626E-10
42	3.210E-10	3.083E-10	3.797E-10
43	3.480E-10	3.380E-10	4.040E-10
44	1.860E-10	1.675E-10	1.773E-10
45	5.190E-10	4.525E-10	2.007E-10
46	5.160E-10	4.810E-10	2.147E-10
47	3.310E-10	2.884E-10	1.892E-10
48	4.140E-10	4.092E-10	2.063E-10
49	1.800E-10	1.739E-10	3.417E-10
50	1.040E-10	1.038E-10	
51	8.390E-11	8.331E-11	1.590E-10
52	1.500E-12	1.559E-12	1.658E-12
53	1.460E-12	1.517E-12	1.614E-12
54	1.420E-12	1.487E-12	1.555E-12
55	2.010E-10	1.859E-10	2.256E-10
56	6.620E-11	8.241E-11	6.025E-11
57	5.560E-11	7.292E-11	5.183E-11
58	1.840E-10	1.493E-10	1.238E-10
59	3.650E-10	3.539E-10	4.308E-10
60	1.130E-10	1.129E-10	8.714E-11
61	3.590E-10	3.486E-10	3.860E-10
62	3.650E-10	3.549E-10	3.931E-10
63	3.660E-10	3.587E-10	3.939E-10

Table 4 – continued

K	τ(CW)	τ(AS)	τ(MCHF)
64	4.600E-11	3.652E-11	5.242E-11
65	1.040E-12	1.076E-12	1.029E-12
66	8.360E-13	8.781E-13	9.415E-13
67	9.300E-13	9.667E-13	1.082E-12
68	6.550E-13	6.971E-13	7.245E-13
69	4.870E-13	5.167E-13	4.932E-13
70	6.730E-13	6.989E-13	7.235E-13
71	5.990E-13	6.196E-13	6.101E-13
72	1.060E-12	1.090E-12	1.574E-12
73	4.880E-13	5.148E-13	5.516E-13
74	8.000E-11	8.110E-11	1.142E-10
75	7.230E-11	7.456E-11	9.349E-11
76	6.530E-13	6.921E-13	8.508E-13
77	7.310E-11	7.449E-11	1.016E-10
78	3.500E-10	3.392E-10	3.712E-10
79	2.610E-11	3.002E-11	2.026E-11
80	1.150E-11	1.189E-11	5.783E-12
81	1.250E-12	1.347E-12	1.339E-12
82	1.560E-12	1.672E-12	1.637E-12
83	4.830E-12	4.982E-12	1.129E-11
84	6.930E-13	7.172E-13	7.888E-13
85	9.960E-13	1.012E-12	1.398E-12
86	5.650E-13	5.981E-13	6.645E-13
87	5.340E-12	7.543E-12	
88	6.250E-13	6.530E-13	6.484E-13
89	5.240E-12	7.373E-12	
90	4.160E-13	4.325E-13	4.780E-13
91	5.230E-12	7.342E-12	
92	3.590E-13	3.750E-13	4.112E-13
93	7.600E-12	8.984E-12	
94	7.600E-12	9.003E-12	
95	7.570E-12	9.000E-12	
96	1.200E-11	1.610E-11	
97	7.800E-12	9.346E-12	
98	1.110E-11	1.413E-11	
99	7.170E-12	7.225E-12	

Table 4 – continued

K	τ(CW)	τ(AS)	τ(MCHF)
100	5.190E-12	5.687E-12	
101	7.840E-12	7.946E-12	
102	3.040E-12	3.466E-12	
103	1.330E-11	2.054E-11	
104	6.640E-12	5.114E-12	
105	2.490E-11	2.525E-11	
106	2.480E-11	2.534E-11	
107	2.470E-11	2.552E-11	
108	2.900E-11	2.647E-11	
109	2.870E-11	2.642E-11	
110	2.850E-11	2.650E-11	
111	1.200E-11	1.217E-11	
112	1.170E-11	1.234E-11	
113	1.210E-11	1.265E-11	
114	7.820E-12	6.568E-12	
115	2.610E-11	2.612E-11	
116	2.520E-11	2.561E-11	
117	2.480E-11	2.550E-11	
118	2.410E-11	2.449E-11	
119	2.500E-11	2.485E-11	
120	2.710E-11	2.771E-11	
121	2.420E-11	2.435E-11	
122	2.430E-11	2.398E-11	
123	3.010E-11	3.229E-11	
124	3.040E-11	3.253E-11	
125	3.260E-11	3.335E-11	
126	1.260E-11	1.317E-11	
127	9.600E-12	1.278E-11	
128	1.240E-11	1.320E-11	
129	6.720E-12	6.853E-12	
130	2.990E-11	2.993E-11	
131	2.480E-11	2.441E-11	
132	2.660E-11	2.747E-11	
133	2.450E-11	2.444E-11	
134	2.430E-11	2.445E-11	
135	2.740E-11	2.529E-11	

Table 4 – continued

K	τ(CW)	τ(AS)	τ(MCHF)
136	2.840E-11	2.816E-11	
137	2.830E-11	2.764E-11	
138	2.760E-11	2.725E-11	
139	2.860E-11	2.678E-11	
140	3.630E-11	3.241E-11	
141	2.500E-10	1.062E-10	
142	9.200E-11	6.756E-11	
143	1.660E-10	8.834E-11	
144	1.340E-11	1.590E-11	
145	1.240E-11	1.469E-11	
146	1.190E-11	1.439E-11	
147	1.940E-11	1.765E-11	
148	1.910E-11	1.777E-11	
149	1.870E-11	1.789E-11	
150	2.290E-11	2.510E-11	
151	1.970E-11	1.647E-11	
152	2.610E-11	2.201E-11	
153	1.290E-11	9.201E-12	
154	8.070E-12	6.723E-12	
155	1.690E-11	9.513E-12	
156	9.280E-12	6.750E-12	

Concerning the radiative lifetimes of the excited levels, we present in Table 4 the calculated values with the HFR and TFDA potential approaches, they differ by less than 11%. They are also compared with the MCHF calculations by Froese Fischer and Tachiev [20, 21].
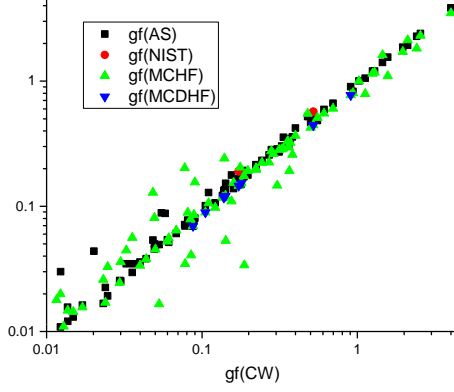
3.2. Transition parameters

Figure 1: Comparison between our calculated values of the weighted oscillator strengths by AS code gf(AS), the values from the NIST database [14] gf(NIST), the MCHF calculated values by Froese Fischer and Tachiev [20, 21] gf(MCHF) and the MCDHF calculated values by Rynkun et al. [5] gf(MCDHF) versus our calculated values by CW code gf(CW).

The two transition parameters that we calculate are oscillator strengths and transition probabilities. We present these calculations in Tables 5 and 6.

Table 5: Weighted oscillator strengths. gf(NIST) are values from the NIST database [14]. gf(CW) and gf(AS) are our calculated values using the CW and AS codes. gf(MCHF) and gf(MCDHF) are respectively, calculated values by Froese Fischer and Tachiev [20, 21] using the MCHF method and by Rynkun et al. [5] using the MCDHF method.

Key	K	K'	gf(NIST)	gf(CW)	gf(AS)	gf(MCHF)	gf(MCDHF)
1	6	1	5.689E-01	5.212E-01	5.022E-01	4.456E-01	4.442E-01
2	6	2	1.905E-01	1.722E-01	1.656E-01	1.462E-01	1.457E-01
3	6	4		5.546E-03	5.182E-03	4.195E-03	4.166E-03
4	7	1		1.799E-01	1.731E-01	1.542E-01	1.538E-01
5	7	2		1.052E-01	1.012E-01	8.961E-02	8.933E-02
6	7	3		1.384E-01	1.329E-01	1.178E-01	1.174E-01
7	7	4		1.928E-04	2.159E-04	1.108E-04	1.132E-04
8	7	5		8.260E-04	9.030E-04	6.408E-04	6.218E-04
9	8	2		1.419E-01	1.366E-01	1.212E-01	1.209E-01
10	9	1		8.511E-03	8.388E-03	6.625E-03	6.572E-03
11	9	2		2.042E-04	1.765E-04	1.889E-04	1.899E-04
12	9	3		5.383E-04	4.273E-04	4.021E-04	3.898E-04
13	9	4		9.078E-01	9.012E-01	7.755E-01	7.718E-01

17

Table 5 – continued

Key	K	K'	gf(NIST)	gf(CW)	gf(AS)	gf(MCHF)	gf(MCDHF)
14	9	5		8.750E-02	6.922E-02	6.970E-02	6.947E-02
15	11	1		6.714E-04	7.738E-04	6.875E-04	
16	11	2		1.469E-04	1.606E-04	1.270E-04	
17	13	1		5.741E-03	5.296E-03	5.595E-03	
18	13	2		6.839E-02	6.067E-02	6.429E-02	
19	13	3		5.998E-02	5.401E-02	5.242E-02	
20	13	4		1.758E-03	1.645E-03	2.095E-03	
21	13	5		4.256E-04	2.808E-04	8.601E-04	
22	14	1		8.872E-02	7.622E-02	8.560E-02	
23	14	2		1.358E-01	1.219E-01	1.182E-01	
24	14	4		5.559E-04	6.695E-06	3.029E-04	
25	15	1		3.133E-01	2.712E-01	2.832E-01	
26	15	4		3.540E-03	3.512E-03	3.475E-03	
27	16	1		1.371E-02	1.204E-02	1.473E-02	
28	16	2		4.775E-03	3.084E-03	5.949E-03	
29	16	4		5.546E-01	4.836E-01	5.105E-01	
30	23	2		4.375E-02	3.807E-02	3.792E-02	
31	24	1		3.990E-02	3.576E-02	3.367E-02	
32	24	2		2.958E-02	2.553E-02	2.445E-02	
33	24	3		6.109E-02	5.148E-02	5.581E-02	
34	24	4		3.784E-03	2.791E-03	3.021E-03	
35	24	5		1.256E-04	7.517E-07	8.370E-05	
36	25	1		1.216E-01	1.064E-01	9.750E-02	
37	25	2		8.453E-02	7.061E-02	7.869E-02	
38	25	4		2.472E-02	1.925E-02	3.291E-02	
39	26	1		6.699E-04	5.429E-04	3.092E-04	
40	26	2		5.984E-05	1.037E-05	1.195E-05	
41	26	3		4.102E-04	2.244E-04	5.887E-04	
42	26	4		1.782E-01	1.493E-01	1.525E-01	
43	26	5		1.600E-01	1.383E-01	1.540E-01	
44	39	2		4.864E-04	4.847E-04	5.433E-04	
45	40	1		7.278E-04	7.430E-04	8.260E-04	
46	40	2		4.266E-04	4.506E-04	4.296E-04	
47	40	3		2.158E-04	1.888E-04	2.752E-04	
48	40	4		5.572E-07	9.642E-07	2.209E-06	
49	40	5		4.046E-08	4.323E-08	2.349E-07	
50	41	1		1.503E-03	1.567E-03	1.544E-03	
51	41	2		3.954E-05	2.010E-05	9.927E-05	
52	41	4		4.581E-07	5.439E-07	1.839E-06	
53	42	1		3.581E-04	4.306E-04	1.883E-04	
54	42	4		7.709E-06	7.806E-06	1.310E-05	
55	52	1		2.432E-01	2.324E-01	2.228E-01	
56	52	2		6.109E-01	5.930E-01	5.514E-01	

Table 5 – continued

Key	K	K'	gf(NIST)	gf(CW)	gf(AS)	gf(MCHF)	gf(MCDHF)
57	52	4		2.244E-03	2.060E-03	1.819E-03	
58	53	1		1.702E-02	1.624E-02	1.564E-02	
59	53	2		2.228E-01	2.147E-01	2.016E-01	
60	53	3		2.884E-01	2.804E-01	2.623E-01	
61	53	4		4.634E-04	4.682E-04	4.452E-04	
62	53	5		6.237E-05	1.159E-04	7.317E-07	
63	54	1		1.253E+00	1.200E+00	1.147E+00	
64	54	4		5.610E-03	5.308E-03	3.631E-03	
65	56	1		4.519E-03	3.439E-03	5.400E-03	
66	56	2		9.078E-03	6.990E-03	1.057E-02	
67	56	4		1.675E-03	1.068E-03	1.704E-03	
68	57	1		2.317E-02	1.672E-02	2.597E-02	
69	57	4		3.112E-03	2.039E-03	3.277E-03	
70	58	2		6.152E-04	9.068E-04	1.367E-03	
71	60	1		2.965E-03	2.511E-03	5.215E-03	
72	60	4		7.709E-03	8.054E-03	1.034E-02	
73	65	1		6.839E-03	5.399E-03	5.090E-02	
74	65	2		7.745E-02	7.115E-02	2.027E-01	
75	65	3		3.055E-01	2.865E-01	1.467E-01	
76	65	4		2.799E-01	2.836E-01	2.759E-01	
77	65	5		5.012E-02	4.659E-02	4.533E-02	
78	66	1		1.549E-01	1.777E-01	1.099E-01	
79	66	2		1.291E+00	1.200E+00	1.175E+00	
80	66	4		1.528E-03	6.891E-04	1.809E-04	
81	67	1		5.309E-02	4.935E-02	1.655E-02	
82	67	2		1.875E-01	1.929E-01	3.393E-02	
83	67	3		1.393E-01	1.352E-01	2.412E-01	
84	67	4		3.707E-01	3.466E-01	3.227E-01	
85	67	5		4.943E-02	4.539E-02	8.105E-02	
86	68	1		2.553E+00	2.397E+00	2.312E+00	
87	68	4		1.368E-02	1.564E-02	7.690E-03	
88	69	1		2.109E+00	1.927E+00	2.128E+00	
89	69	2		3.342E-01	3.556E-01	2.902E-01	
90	69	4		1.233E-02	3.004E-02	2.612E-03	
91	70	2		3.565E-01	3.434E-01	3.315E-01	
92	71	1		4.797E-01	5.204E-01	5.500E-01	
93	71	2		3.622E-01	3.020E-01	2.958E-01	
94	71	3		3.258E-01	3.027E-01	2.864E-01	
95	71	4		3.258E-02	3.476E-02	4.454E-02	
96	71	5		1.493E-04	4.263E-04	5.247E-04	
97	72	1		5.483E-02	8.860E-02	3.065E-03	
98	72	2		9.840E-04	4.497E-04	2.738E-03	
99	72	4		1.125E+00	1.054E+00	7.900E-01	

Table 5 – continued

Key	K	K'	gf(NIST)	gf(CW)	gf(AS)	gf(MCHF)	gf(MCDHF)
100	73	1		9.376E-01	8.269E-01	8.035E-01	
101	73	2		3.999E-01	4.208E-01	3.666E-01	
102	73	3		1.104E-01	1.287E-01	1.060E-01	
103	73	4		1.288E-02	9.019E-03	1.097E-02	
104	73	5		1.416E-03	7.904E-04	3.841E-03	
105	76	1		2.228E-01	2.024E-01	1.962E-01	
106	76	4		2.410E+00	2.280E+00	1.825E+00	
107	79	1		2.153E-04	1.719E-04	3.279E-04	
108	79	2		1.230E-02	1.085E-02	1.992E-02	
109	79	4		2.999E-02	2.532E-02	3.593E-02	
110	80	1		8.995E-02	8.042E-02	1.556E-01	
111	80	4		4.842E-02	5.366E-02	1.287E-01	
112	81	2		1.862E-01	1.722E-01	1.751E-01	
113	82	1		4.943E-02	4.987E-02	7.755E-03	
114	82	2		1.762E-01	1.670E-01	2.047E-01	
115	82	3		1.977E-01	1.777E-01	1.923E-01	
116	82	4		1.486E-02	1.307E-02	1.440E-02	
117	82	5		9.268E-03	9.221E-03	1.194E-02	
118	83	1		1.422E-01	1.527E-01	5.315E-02	
119	83	2		8.511E-02	7.052E-02	4.074E-02	
120	83	4		9.226E-03	5.338E-03	8.020E-03	
121	84	1		2.704E-01	2.571E-01	2.243E-01	
122	84	2		1.026E+00	1.004E+00	9.996E-01	
123	84	4		3.828E-01	3.583E-01	2.592E-01	
124	85	1		1.570E+00	1.549E+00	1.097E+00	
125	85	4		3.565E-02	2.966E-02	5.615E-02	
126	86	1		2.393E-02	2.248E-02	1.706E-02	
127	86	2		5.012E-01	4.668E-01	4.251E-01	
128	86	3		6.982E-01	6.642E-01	6.041E-01	
129	86	4		1.172E-03	1.039E-03	9.975E-04	
130	86	5		1.384E-03	3.684E-04	2.204E-03	
131	88	1		7.798E-02	6.954E-02	3.478E-02	
132	88	2		3.656E-01	3.308E-01	1.925E-01	
133	88	4		1.452E+00	1.410E+00	1.619E+00	
134	90	1		1.159E-02	8.990E-03	1.786E-02	
135	90	4		3.999E+00	3.835E+00	3.499E+00	
136	92	1		6.934E-06	1.996E-05	1.060E-06	
137	92	2		2.018E-03	1.441E-03	1.442E-03	
138	92	3		3.296E-04	5.314E-05	1.639E-03	
139	92	4		8.091E-02	7.737E-02	8.915E-02	
140	92	5		1.963E+00	1.863E+00	1.716E+00	
141	103	1		3.034E-03	1.547E-04		
142	103	2		5.224E-03	3.262E-05		

Table 5 – continued

Key	K	K'	gf(NIST)	gf(CW)	gf(AS)	gf(MCHF)	gf(MCDHF)
143	103	4		1.256E-02	1.810E-07		
144	104	1		2.018E-02	4.374E-02		
145	104	2		2.999E-02	2.526E-02		
146	104	3		9.528E-05	8.623E-03		
147	104	4		2.541E-04	2.049E-04		
148	104	5		2.075E-06	3.805E-06		
149	113	1		3.614E-02	3.469E-02		
150	113	4		4.121E-04	5.617E-04		
151	114	1		5.272E-04	9.333E-04		
152	114	2		7.362E-03	7.938E-04		
153	114	4		5.794E-02	8.764E-02		
154	126	2		4.375E-03	4.335E-03		
155	127	1		2.495E-03	3.775E-03		
156	127	2		2.188E-03	2.859E-03		
157	127	3		4.217E-03	5.606E-03		
158	127	4		9.661E-03	1.513E-03		
159	127	5		7.499E-03	3.963E-04		

Table 6: Weighted transition probabilities. gA(NIST) are values from the NIST database [14]. gA(CW) and gA(AS) are our calculated values using the CW and AS codes. gA(MCHF) and gA(MCDHF) are respectively, calculated values by Froese Fischer and Tachiev [20, 21] using the MCHF method and by Rynkun et al. [5] using the MCDHF method.

Key	K	K'	gA(NIST)	gA(CW)	gA(AS)	gA(MCHF)	gA(MCDHF)
1	6	1	9.000E+10	8.24E+10	7.95E+10	7.09E+10	7.030E+10
2	6	2	2.800E+10	2.60E+10	2.50E+10	2.22E+10	2.205E+10
3	6	4		6.59E+08	6.16E+08	5.01E+08	4.954E+08
4	7	1		2.96E+10	2.84E+10	2.55E+10	2.529E+10
5	7	2		1.65E+10	1.59E+10	1.42E+10	1.406E+10
6	7	3		2.15E+10	2.06E+10	1.84E+10	1.822E+10
7	7	4		2.39E+07	2.68E+07	1.38E+07	1.407E+07
8	7	5		7.18E+07	7.92E+07	5.63E+07	5.406E+07
9	8	2		2.28E+10	2.19E+10	1.96E+10	1.944E+10
10	9	1		2.64E+09	2.75E+09	2.01E+09	1.986E+09
11	9	2		6.13E+07	5.61E+07	5.56E+07	5.556E+07
12	9	3		1.60E+08	1.35E+08	1.17E+08	1.129E+08
13	9	4		2.31E+11	2.44E+11	1.92E+11	1.904E+11
14	9	5		1.75E+10	1.49E+10	1.36E+10	1.340E+10
15	11	1		1.99E+09	2.28E+09	2.03E+09	
16	11	2		4.30E+08	4.68E+08	3.72E+08	
17	13	1		1.86E+10	1.71E+10	1.81E+10	

Table 6 – continued

Key	K	K'	gA(NIST)	gA(CW)	gA(AS)	gA(MCHF)	gA(MCDHF)
18	13	2		2.19E+11	1.94E+11	2.06E+11	
19	13	3		1.91E+11	1.72E+11	1.67E+11	
20	13	4		5.35E+09	5.01E+09	6.38E+09	
21	13	5		1.21E+09	8.00E+08	2.45E+09	
22	14	1		2.87E+11	2.46E+11	2.77E+11	
23	14	2		4.35E+11	3.90E+11	3.79E+11	
24	14	4		1.69E+09	2.04E+07	9.23E+08	
25	15	1		1.01E+12	8.78E+11	9.17E+11	
26	15	4		1.08E+10	1.07E+10	1.06E+10	
27	16	1		4.49E+10	3.95E+10	4.83E+10	
28	16	2		1.55E+10	1.00E+10	1.93E+10	
29	16	4		1.71E+12	1.49E+12	1.58E+12	
30	23	2		1.48E+11	1.29E+11	1.27E+11	
31	24	1		1.36E+11	1.22E+11	1.14E+11	
32	24	2		1.00E+11	8.65E+10	8.19E+10	
33	24	3		2.06E+11	1.74E+11	1.86E+11	
34	24	4		1.22E+10	9.00E+09	9.63E+09	
35	24	5		3.79E+08	2.28E+06	2.50E+08	
36	25	1		4.16E+11	3.64E+11	3.31E+11	
37	25	2		2.87E+11	2.40E+11	2.64E+11	
38	25	4		7.99E+10	6.22E+10	1.05E+11	
39	26	1		2.32E+09	1.88E+09	1.06E+09	
40	26	2		2.05E+08	3.56E+07	4.06E+07	
41	26	3		1.40E+09	7.69E+08	2.00E+09	
42	26	4		5.82E+11	4.89E+11	4.94E+11	
43	26	5		4.91E+11	4.25E+11	4.67E+11	
44	39	2		1.83E+09	1.81E+09	2.05E+09	
45	40	1		2.77E+09	2.81E+09	3.14E+09	
46	40	2		1.61E+09	1.69E+09	1.62E+09	
47	40	3		8.11E+08	7.05E+08	1.03E+09	
48	40	4		2.00E+06	3.45E+06	7.94E+06	
49	40	5		1.37E+05	1.45E+05	7.94E+05	
50	41	1		5.72E+09	5.92E+09	5.87E+09	
51	41	2		1.49E+08	7.53E+07	3.74E+08	
52	41	4		1.65E+06	1.94E+06	6.61E+06	
53	42	1		1.36E+09	1.63E+09	7.15E+08	
54	42	4		2.77E+07	2.79E+07	4.71E+07	
55	52	1		9.48E+11	9.03E+11	8.68E+11	
56	52	2		2.36E+12	2.28E+12	2.13E+12	
57	52	4		8.30E+09	7.58E+09	6.71E+09	
58	53	1		6.65E+10	6.31E+10	6.09E+10	
59	53	2		8.61E+11	8.27E+11	7.78E+11	
60	53	3		1.11E+12	1.08E+12	1.01E+12	

Table 6 – continued

Key	K	K'	gA(NIST)	gA(CW)	gA(AS)	gA(MCHF)	gA(MCDHF)
61	53	4		1.71E+09	1.72E+09	1.64E+09	
62	53	5		2.17E+08	4.02E+08	2.54E+06	
63	54	1		4.90E+12	4.67E+12	4.47E+12	
64	54	4		2.07E+10	1.95E+10	1.34E+10	
65	56	1		1.84E+10	1.40E+10	2.20E+10	
66	56	2		3.67E+10	2.82E+10	4.27E+10	
67	56	4		6.48E+09	4.12E+09	6.58E+09	
68	57	1		9.45E+10	6.81E+10	1.06E+11	
69	57	4		1.21E+10	7.88E+09	1.27E+10	
70	58	2		2.49E+09	3.67E+09	5.54E+09	
71	60	1		1.22E+10	1.03E+10	2.15E+10	
72	60	4		3.00E+10	3.13E+10	4.03E+10	
73	65	1		2.83E+10	2.23E+10	2.12E+11	
74	65	2		3.18E+11	2.92E+11	8.36E+11	
75	65	3		1.25E+12	1.17E+12	6.03E+11	
76	65	4		1.10E+12	1.11E+12	1.09E+12	
77	65	5		1.85E+11	1.73E+11	1.69E+11	
78	66	1		6.44E+11	7.38E+11	4.57E+11	
79	66	2		5.31E+12	4.94E+12	4.84E+12	
80	66	4		6.02E+09	2.71E+09	7.13E+08	
81	67	1		2.21E+11	2.05E+11	6.85E+10	
82	67	2		7.72E+11	7.94E+11	1.39E+11	
83	67	3		5.73E+11	5.55E+11	9.88E+11	
84	67	4		1.46E+12	1.37E+12	1.27E+12	
85	67	5		1.84E+11	1.69E+11	3.00E+11	
86	68	1		1.06E+13	9.95E+12	9.61E+12	
87	68	4		5.39E+10	6.16E+10	3.03E+10	
88	69	1		8.82E+12	8.07E+12	8.91E+12	
89	69	2		1.39E+12	1.48E+12	1.20E+12	
90	69	4		4.90E+10	1.19E+11	1.04E+10	
91	70	2		1.48E+12	1.43E+12	1.38E+12	
92	71	1		2.01E+12	2.18E+12	2.31E+12	
93	71	2		1.50E+12	1.25E+12	1.23E+12	
94	71	3		1.35E+12	1.25E+12	1.19E+12	
95	71	4		1.30E+11	1.38E+11	1.77E+11	
96	71	5		5.60E+08	1.60E+09	1.97E+09	
97	72	1		2.30E+11	3.72E+11	1.28E+10	
98	72	2		4.10E+09	1.87E+09	1.14E+10	
99	72	4		4.48E+12	4.20E+12	3.14E+12	
100	73	1		3.95E+12	3.48E+12	3.39E+12	
101	73	2		1.67E+12	1.76E+12	1.53E+12	
102	73	3		4.60E+11	5.36E+11	4.42E+11	
103	73	4		5.14E+10	3.61E+10	4.39E+10	

Table 6 – continued

Key	K	K'	gA(NIST)	gA(CW)	gA(AS)	gA(MCHF)	gA(MCDHF)
104	73	5		5.34E+09	2.98E+09	1.45E+10	
105	76	1		9.48E+11	8.63E+11	8.35E+11	
106	76	4		9.76E+12	9.23E+12	7.37E+12	
107	79	1		9.29E+08	7.42E+08	1.41E+09	
108	79	2		5.26E+10	4.65E+10	8.47E+10	
109	79	4		1.23E+11	1.04E+11	1.46E+11	
110	80	1		3.88E+11	3.47E+11	6.67E+11	
111	80	4		1.98E+11	2.20E+11	5.24E+11	
112	81	2		7.99E+11	7.39E+11	7.45E+11	
113	82	1		2.14E+11	2.16E+11	3.33E+10	
114	82	2		7.56E+11	7.17E+11	8.72E+11	
115	82	3		8.47E+11	7.61E+11	8.17E+11	
116	82	4		6.11E+10	5.38E+10	5.87E+10	
117	82	5		3.60E+10	3.59E+10	4.60E+10	
118	83	1		6.16E+11	6.62E+11	2.29E+11	
119	83	2		3.66E+11	3.03E+11	1.74E+11	
120	83	4		3.80E+10	2.20E+10	3.28E+10	
121	84	1		1.18E+12	1.12E+12	9.71E+11	
122	84	2		4.44E+12	4.35E+12	4.29E+12	
123	84	4		1.59E+12	1.49E+12	1.07E+12	
124	85	1		6.86E+12	6.77E+12	4.76E+12	
125	85	4		1.48E+11	1.23E+11	2.31E+11	
126	86	1		1.05E+11	9.84E+10	7.40E+10	
127	86	2		2.17E+12	2.03E+12	1.83E+12	
128	86	3		3.02E+12	2.88E+12	2.59E+12	
129	86	4		4.87E+09	4.32E+09	4.11E+09	
130	86	5		5.43E+09	1.45E+09	8.57E+09	
131	88	1		3.42E+11	3.06E+11	1.52E+11	
132	88	2		1.59E+12	1.44E+12	8.33E+11	
133	88	4		6.06E+12	5.89E+12	6.71E+12	
134	90	1		5.11E+10	3.98E+10	7.82E+10	
135	90	4		1.68E+13	1.61E+13	1.45E+13	
136	92	1		3.13E+07	9.03E+07	4.74E+06	
137	92	2		9.03E+09	6.47E+09	6.39E+09	
138	92	3		1.47E+09	2.38E+08	7.25E+09	
139	92	4		3.47E+11	3.33E+11	3.79E+11	
140	92	5		7.96E+12	7.59E+12	6.89E+12	
141	103	1		1.70E+10	8.38E+08		
142	103	2		2.91E+10	1.75E+08		
143	103	4		6.73E+10	9.36E+05		
144	104	1		1.14E+11	2.38E+11		
145	104	2		1.67E+11	1.37E+11		
146	104	3		5.31E+08	4.66E+10		

Table 6 – continued

Key	K	K'	gA(NIST)	gA(CW)	gA(AS)	gA(MCHF)	gA(MCDHF)
147	104	4		1.37E+09	1.07E+09		
148	104	5		1.06E+07	1.88E+07		
149	113	1		2.10E+11	2.01E+11		
150	113	4		2.29E+09	3.11E+09		
151	114	1		3.07E+09	5.42E+09		
152	114	2		4.25E+10	4.57E+09		
153	114	4		3.23E+11	4.87E+11		
154	126	2		2.62E+10	2.60E+10		
155	127	1		1.51E+10	2.28E+10		
156	127	2		1.31E+10	1.71E+10		
157	127	3		2.53E+10	3.35E+10		
158	127	4		5.59E+10	8.74E+09		
159	127	5		4.14E+10	2.18E+09		

Computed transition rates are in close agreement with available data from MCHF calculations by Froese Fischer and Tachiev [20, 21] and MCDHF calculations by Rynkun et al. [5].

To see the difference between the different transition parameters, we plot in Figure 1 the weighted oscillator strengths calculated by AS and those from the NIST database [14], from Froese Fischer and Tachiev [20, 21] using the MCHF method and from Rynkun et al. [5] using the MCDHF method, versus the CW values.

In the NIST-ASD database there are only two values that we put in the Figure 1 (in red color circle). The CW, AS, MCHF and MCDHF values are 9.0%, 12.4%, 22.5% and 22.7% from the NIST-ASD values. The 14 MCDHF gf values are less than 1% different from the MCHF values.

Comparing the 140 gf values from CW, AS and MCHF, we notice that the AS and MCHF values are 20% and 48% respectively far from those of the CW.

4. Conclusions

In this work, within the framework of the HFR and TFDA methods, a consistent atomic data set including energy levels, lifetimes and transition data are provided for the lowest states for the O-like Cl X ion. Energy levels and radiative lifetimes are provided for the 156 lowest levels belonging to the 10 configurations $2s^a2p^{6-a}$ (a=0-2), $2s^22p^33l$ (ℓ=0-2), $2s^22p^34l$ (ℓ=0,1) and $2s^22p^3ns$ (n=3,4).

Oscillator strengths and transition probabilities for 159 transitions are calculated. They are in agreement with the results from other calculations and available measurements for most of the considered transitions.

The new results of this work are important for fusion plasma and astrophysical applications.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

References

[1] P. Bogdanovich, R. Karpuškiene, I. Martinson, Ab initio wavelengths and oscillator strengths for Cl X, Physica Scripta 67 (1) (2003) 44.

[2] C. J. Fontes, H. L. Zhang, Relativistic distorted-wave collision strengths for the 16 $\Delta n = 0$ optically allowed transitions with n= 2 in the 67 O-like ions with $26 \leq Z \leq 92$, Atomic Data and Nuclear Data Tables 101 (2015) 143–157.

[3] P. Bogdanovich, D. Majus, T. Pakhomova, Investigation of accuracy of configuration interaction for the oxygen isoelectronic sequence, Physica Scripta 74 (5) (2006) 558.

[4] S. Yong, W. Rong, J. Gang, Z. Zheng-he, Calculation of the fine structure of oxygen-like ions using polarization potential function, Chinese Physics 10 (6) (2001) 505.

[5] P. Rynkun, P. Jönsson, G. Gaigalas, C. F. Fischer, Energies and E1, M1, E2, and M2 transition rates for states of the $2s^2 2p^4$, $2s2p^5$, and $2p^6$ configurations in oxygen-like ions between F II and Kr XXIX, Astronomy & Astrophysics 557 (2013) A136.

[6] A. Al-Modlej, R. A. B. Alraddadi, N. Ben Nessib, Energy levels and oscillator strengths for carbon isoelectronic sequence from C I to Ne V, The European Physical Journal Plus 133 (9) (2018) 1.

[7] R. D. Cowan, The theory of atomic structure and spectra, Univ. of California Press, 1981.

[8] A. Kramida, A suite of atomic structure codes originally developed by r. d. cowan adapted for windows-based personal computers., Public Data Resource/National Institute of Standards and Technology (2021). doi:https://doi.org/10.18434/T4/1502500. URL https://data.nist.gov/od/id/6CF509047B474AC9E05324570681DE731930

[9] W. Eissner, M. Jones, H. Nussbaumer, Techniques for the calculation of atomic structures and radiative data including relativistic corrections, Computer Physics Communications 8 (4) (1974) 270.

[10] N. R. Badnell, Dielectronic recombination of Fe^{22+} and Fe^{21+}, Journal of Physics B: Atomic and Molecular Physics 19 (1986) 3827–3835.

[11] A. Almodlej, H. Alrashed, N. Ben Nessib, M. S. Dimitrijević, Atomic structure for carbon-like ions from Na VI to Ar XIII, Monthly Notices of the Royal Astronomical Society 507 (3) (2021) 3228–3237.

[12] N. Alwadie, A. Almodlej, N. Ben Nessib, M. S. Dimitrijević, Atomic structure of the carbon like ion Ca XV, Contrib. Astron. Obs. Skalnaté Pleso 50 (2020) 86–95.

[13] C. Froese Fischer, G. Gaigalas, P. Jönsson, J. Biero, GRASP2018a Fortran 95 version of the general relativistic atomic structure package, Computer Physics Communications 237 (2019) 184–187.

[14] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team, NIST Atomic Spectra Database (ver. 5.10), [Online]. Available: https://physics.nist.gov/asd [2023, December 13]. National Institute of Standards and Technology, Gaithersburg, MD. (2023).

[15] L. Abu El Maati, A. Mahmoud, I. S. Mahmoud, S. G. Tawfik, N. Alwadii, N. Ben Nessib, M. S. Dimitrijević, Atomic structure and transition parameters of the V XVIII carbon-like ion, Contrib. Astron. Obs. Skalnaté Pleso 52 (3) (2022) 44–70.

[16] N. R. Badnell, A BreitPauli distorted wave implementation for autostructure, Computer Physics Communications 182 (7) (2011) 1528–1535.

[17] H. Nussbaumer, P. Storey, Bound-bound radiative transitions in C I, Astronomy and Astrophysics 140 (1984) 383–389.

[18] N. Badnell, On the effects of the two-body non-fine-structure operators of the Breit-Pauli hamiltonian, Journal of Physics B: Atomic, Molecular and Optical Physics 30 (1) (1997) 1.

[19] C. Zeippen, M. Seaton, D. Morton, Some O I oscillator strengths and the interstellar abundance of oxygen, Monthly Notices of the Royal Astronomical Society 181 (3) (1977) 527.

[20] C. F. Fischer, G. Tachiev, Breit–Pauli energy levels, lifetimes, and transition probabilities for the beryllium-like to neon-like sequences, Atomic Data and Nuclear Data Tables 87 (1) (2004) 1–184.

[21] C. F. Fischer, G. Tachiev, MCHF/MCDHF collection, version 2 (June, 2009).
URL http://physics.nist.gov/mchf