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Research Article

Atomic Structure Calculations for Neutral Oxygen

Norah Alonizan, Rabia Qindeel, and Nabil Ben Nessib

Department of Physics and Astronomy, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

Correspondence should be addressed to Nabil Ben Nessib; nbennessib@ksu.edu.sa

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Energy levels and oscillator strengths for neutral oxygen have been calculated using the Cowan (CW), SUPERSTRUCTURE (SS), and AUTOSTRUCTURE (AS) atomic structure codes. The results obtained with these atomic codes have been compared with MCHF calculations and experimental values from the National Institute of Standards and Technology (NIST) database.

1. Introduction

Oxygen atom (O I) is the most abundant element after hydrogen and helium in the Universe. Its spectroscopic study is very important for the knowledge of the structure of stars, galaxies and in general the whole Universe. It is also important for studying the life on the earth and the possibility of life on other planets or exoplanets. The studies of earth's atmosphere and its radiative properties need these data. Industrial and technical applications need the characteristics of this element.

Pradhan and Saraph [1] calculated oscillator strengths for dipole transitions in O I using the SUPERSTRUCTURE (SS) code [2] with spectroscopic type orbitals for 1s, 2s, and 2p and correlation type orbitals for the $\overline{3d}$. Tayal and Henry [3] calculated oscillator strengths and electron collisional excitation cross sections for O I. They used the Hibbert CIV3 atomic structure code [4] with the eight orthogonal one-electron orbitals 1s, 2s, 2p, 3s, 3p, 3d, 4s, and 4p. Using the same CIV3 atomic structure code, Bell and Hibbert [5] calculated oscillator strengths for allowed transitions in O I with more single electron orbitals. Hibbert et al. (HBGV) [6] used the CIV3 code to calculate E1 transitions connecting the $n = 3$ and $n = 4$ energy levels in O I. Biémont et al. [7] calculate oscillator strengths of astrophysical interest for O I using the CIV3 configuration interaction code and the Hartree-Fock pseudorelativistic (HFR) suite of Cowan (CW) codes [8]. Using the SS code, Biémont and Zeippen [9] calculated oscillator strengths for $2p^4$-3s and 3s-3p allowed or spin-forbidden transitions in O I. Zheng and Wang [10] used the Weakest Bound Electron Potential Model (WBEPM) theory to calculate radiative lifetime, transition probabilities, and oscillator strengths for atomic carbon and oxygen. Using the Multiconfiguration Hartree-Fock (MCHF) method [11], Tachiev and Froese Fischer (TFF) [12] calculated *ab initio* Breit-Pauli energy levels and transition rates for nitrogen-like and oxygen-like sequences. Froese Fischer and Tachiev (FFT) [13] calculated Breit-Pauli energy levels, lifetimes, and transition probabilities for the beryllium-like to neon-like sequences in the adjusted with experimental values. Fan et al. [14] used the WBEPMT theory to calculate energy levels of high states in O I. Çelik and Ateş [15] employed the WBEPMT theory to calculate radial transition matrix elements and then atomic transition probabilities for O I.

Using CW or SS or AS codes, we did atomic structure calculations for several atoms and ions [16–18] that are needed for *ab initio* Stark broadening calculations [19, 20] and for emission line ratio calculations [21], but we never compare results obtained by the three codes for the same element.

About O I atomic data in databases, we used the National Institute of Standards and Technology (NIST) data [22] for fine structure energy levels and oscillator strengths. There are energy levels and oscillator strengths of O I without fine structure in the Opacity Project TOPbase [23] and NORAD-Atomic-Data [24] atomic structure databases. TIPbase database [25] of the Opacity Project used NIST data for the fine structure energy levels and Galavis et al. [26] data for the oscillator strengths fine structure data. Galavis et al. [26] used the SS atomic structure code with spectroscopic type

Table 1: The scaling parameters used after minimization for the SS and AS atomic structure codes.

Scaling parameters	1s	2s	2p	3s	3p	3d	4s
$\lambda_{n\ell}$ (SS)	1.23103	1.23103	1.15865	1.23103	1.15865	0.92431	1.23103
$\lambda_{n\ell}$ (AS)	1.55498	1.16135	1.20894	1.07693	2.38871	0.91505	2.33806

orbitals for 1s, 2s, and 2p and correlation type orbitals for $\overline{3s}$, $\overline{3p}$, $\overline{3d}$, and $\overline{4f}$.

In the Chianti project [27], they used the NIST database for experimental energy levels and oscillator strengths. For theoretical energy levels they used the Zatsarinny and Tayal [28] and FFT [13] for the theoretical oscillator strengths.

In this work, we will calculate atomic data for transitions with fine structure in O I using CW and SS and AS codes. Comparison with other theoretical and experimental data available in the literature will be presented.

2. Methods for Calculation

2.1. Hartree-Fock Pseudorelativistic (HFR) Method. In this method a set of orbitals are obtained for each electron configuration by solving the Hartree-Fock equations [8]. A totally antisymmetric wave-function is a combination of single electron solution of the hydrogen atom Ψ (Slater determinant):

$$\Psi = \frac{1}{\sqrt{N}} \begin{vmatrix} \psi_1(1) & \psi_1(2) & \cdots & \psi_1(N) \\ \psi_2(1) & \psi_2(2) & \cdots & \psi_2(N) \\ \cdots & \cdots & \cdots & \cdots \\ \psi_N(1) & \psi_N(2) & \cdots & \psi_N(N) \end{vmatrix}. \quad (1)$$

$\psi_j(i)$ means that the ith electron's space and spin are in the one-electron state ψ_j. This will automatically satisfy the Pauli principle, because a determinant vanishes if two columns are the same.

Relativistic corrections are introduced by a Breit-Pauli Hamiltonian and treated by the perturbation theory. The relativistic corrections include the Blume-Watson spin-orbit, mass-variation, and one-body Darwin terms. The Blume-Watson spin-orbit term contains the part of the Breit interaction that can be reduced to a one-body operator.

The Cowan (CW) atomic structure suite of codes (RCN, RNC2, RCG, and RCE) uses this HFR method. The three first codes are for *ab initio* atomic structure calculations and the fourth one (RCE) is used to make least-squares fit calculations using an iterative procedure.

2.2. Thomas-Fermi-Dirac-Amaldi (TFDA) Method. In this method and to have atomic parameters of an atom or ion, a statistical TFDA potential is used. For an atom or ion having Z protons and N electrons, this potential is in the following form [29]:

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

where

$$\phi(x) = e^{-Zr/2} + \lambda_{n\ell}\left(1 - e^{-Zr/2}\right), \quad x = \frac{r}{\mu} \quad (3)$$

with μ the constant:

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

and $\lambda_{n\ell}$ are the orbital scaling parameters.

The function ϕ verifies the following equation:

$$\frac{d^2\phi}{dx^2} = \frac{1}{\sqrt{x}}\phi(x)^{3/2} \quad (5)$$

with the boundary conditions:

$$\phi(0) = 1, \qquad \phi(\infty) = -\frac{Z-N+1}{Z}. \quad (6)$$

The SUPERSTRUCTURE (SS) and AUTOSTRUCTURE (AS) atomic structure codes use this method. Relativistic corrections are also done by a perturbation method using the Breit-Pauli Hamiltonian. The SS atomic structure code used in this work [30] is an updated version of the original one of 1974 [2]. Some relativistic corrections are introduced in this version and orbital scaling parameters $\lambda_{n\ell}$ are dependent on n and ℓ [31] and not like the original SS version of 1974, where scaling parameters were depending only on ℓ (λ_ℓ). The AS code [32, 33] 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. Comparing the two atomic structure codes SS and AS we can see that even they used the same techniques in general; they gave different results mainly because they incorporated different relativistic corrections of the Hamiltonian. For the comparison between the two codes, we can refer to the work of Elabidi and Sahal-Bréchot [34] where they studied excitation cross section by electron impact for O V and O VI levels. They showed that the incorporation of the two-body non-fine-structure operators (contact spin-spin, two-body Darwin, and orbit-orbit) in AS and not in the initial SS code is the main reason of the different results obtained by the two codes.

Table 2: Energy levels for configuration $2s^2\,2p^4$. E(NIST) are from NIST database [22]. E(CW), E(SS), and E(AS) are energy levels calculated using, respectively, the Cowan, SUPERSTRUCTURE, and AUTOSTRUCTURE atomic codes. E(TFF) are energy levels values from Tachiev and Froese Fisher [12]. All energies are in cm^{-1}.

Configuration	Term	J	E(NIST)	E(CW)	E(SS)	E(AS)	E(TFF)
$2s^22p^4$	^3P	2	0	0	0	0	0
$2s^22p^4$	^3P	1	158	141	171	204	156
$2s^22p^4$	^3P	0	227	210	255	303	223
$2s^22p^4$	^1D	2	15868	14941	18881	17364	16122
$2s^22p^4$	^1S	0	33793	37013	45746	42140	33844

Table 3: The same as Table 2 for configuration $2s^2\,2p^3\,3s$.

Configuration	Term	J	E(NIST)	E(CW)	E(SS)	E(AS)	E(TFF)
$2s^22p^3(^4S^\circ)3s$	$^5S^\circ$	2	73768	70285	50342	67409	74012
$2s^22p^3(^4S^\circ)3s$	$^3S^\circ$	1	76795	72704	54546	70365	76910
$2s^22p^3(^2D^\circ)3s$	$^3D^\circ$	3	101135	96475	80769	99037	—
$2s^22p^3(^2D^\circ)3s$	$^3D^\circ$	2	101148	96474	80768	99036	—
$2s^22p^3(^2D^\circ)3s$	$^3D^\circ$	1	101155	96473	80767	99035	—
$2s^22p^3(^2D^\circ)3s$	$^1D^\circ$	2	102662	97684	82871	100502	—
$2s^22p^3(^2P^\circ)3s$	$^3P^\circ$	2	113911	113471	100024	119170	—
$2s^22p^3(^2P^\circ)3s$	$^3P^\circ$	1	113921	113469	100023	119169	—
$2s^22p^3(^2P^\circ)3s$	$^3P^\circ$	0	113928	113468	100022	119168	—
$2s^22p^3(^2P^\circ)3s$	$^1P^\circ$	1	115918	114666	101453	121545	—

Table 4: The same as Table 2 for configuration $2s^2\,2p^3\,3p$ except that we did not put the AS data because they are too far from the other results.

Configuration	Term	J	E(NIST)	E(CW)	E(SS)	E(TFF)
$2s^22p^3(^4S^\circ)3p$	^5P	1	86626	83148	62276	86645
$2s^22p^3(^4S^\circ)3p$	^5P	2	86628	83149	62279	86647
$2s^22p^3(^4S^\circ)3p$	^5P	3	86631	83152	62284	86650
$2s^22p^3(^4S^\circ)3p$	^3P	1	88631	85516	67495	88590
$2s^22p^3(^4S^\circ)3p$	^3P	2	88631	85519	67492	88591
$2s^22p^3(^4S^\circ)3p$	^3P	0	88631	85514	67497	88591
$2s^22p^3(^2D^\circ)3p$	^1P	1	113204	108935	91748	—
$2s^22p^3(^2D^\circ)3p$	^3D	3	113295	108877	91674	—
$2s^22p^3(^2D^\circ)3p$	^3D	2	113295	108871	91665	—
$2s^22p^3(^2D^\circ)3p$	^3D	1	113298	108864	91655	—
$2s^22p^3(^2D^\circ)3p$	^3F	4	113714	109075	92012	—
$2s^22p^3(^2D^\circ)3p$	^3F	3	113721	109072	92007	—
$2s^22p^3(^2D^\circ)3p$	^3F	2	113727	109069	92003	—
$2s^22p^3(^2D^\circ)3p$	^1F	3	113996	109318	92419	—
$2s^22p^3(^2D^\circ)3p$	^1D	2	116631	113447	101312	—
$2s^22p^3(^2P^\circ)3p$	^3D	3	127283	126148	111485	—
$2s^22p^3(^2P^\circ)3p$	^3D	2	127288	126149	111486	—
$2s^22p^3(^2P^\circ)3p$	^3D	1	127292	126149	111485	—
$2s^22p^3(^2P^\circ)3p$	^1P	1	127668	126335	111820	—
$2s^22p^3(^2P^\circ)3p$	^1D	2	128595	127944	115611	—
$2s^22p^3(^2P^\circ)3p$	^1S	0	130943	132423	111145	—
$2s^22p^3(^2D^\circ)3p$	^3P	1	—	111274	96720	—
$2s^22p^3(^2D^\circ)3p$	^3P	2	—	111280	96730	—
$2s^22p^3(^2D^\circ)3p$	^3P	0	—	111272	96715	—
$2s^22p^3(^2P^\circ)3p$	^3P	1	—	127427	113836	—
$2s^22p^3(^2P^\circ)3p$	^3P	2	—	127418	113812	—
$2s^22p^3(^2P^\circ)3p$	^3P	0	—	127432	113848	—

Table 5: The same as Table 2 for configuration $2s^2\ 2p^3\ 3d$.

Configuration	Term	J	E(NIST)	E(CW)	E(SS)	E(AS)	E(TFF)
$2s^22p^3(^4S^\circ)3d$	$^5D^\circ$	4	97421	94227	72721	89755	97147
$2s^22p^3(^4S^\circ)3d$	$^5D^\circ$	3	97421	94227	72721	89755	97147
$2s^22p^3(^4S^\circ)3d$	$^5D^\circ$	2	97421	94227	72721	89755	97147
$2s^22p^3(^4S^\circ)3d$	$^5D^\circ$	1	97421	94227	72721	89755	97147
$2s^22p^3(^4S^\circ)3d$	$^5D^\circ$	0	97421	94227	72721	89754	97148
$2s^22p^3(^4S^\circ)3d$	$^3D^\circ$	1	97488	94299	72820	89836	97205
$2s^22p^3(^4S^\circ)3d$	$^3D^\circ$	2	97488	94299	72820	89836	97205
$2s^22p^3(^4S^\circ)3d$	$^3D^\circ$	3	97489	94299	72821	89836	97205
$2s^22p^3(^2D^\circ_{3/2})3d$	$^3P^\circ$	2	123297	120045	102401	120957	—
$2s^22p^3(^2D^\circ_{3/2})3d$	$^3P^\circ$	1	123356	120049	102405	120959	—
$2s^22p^3(^2D^\circ_{3/2})3d$	$^3P^\circ$	0	123387	120050	102406	120961	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^3F^\circ$	4	124214	119938	102042	120523	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^3F^\circ$	3	124219	119935	102039	120520	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^3F^\circ$	2	124224	119934	102037	120518	—
$2s^22p^3(^2D^\circ)3d$	$^3G^\circ$	4	124239	119945	102051	120530	—
$2s^22p^3(^2D^\circ)3d$	$^3G^\circ$	5	124240	119946	102053	120531	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^1S^\circ$	0	124243	119935	102037	120519	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^3D^\circ$	3	124247	119957	102070	120544	—
$2s^22p^3(^2D^\circ)3d$	$^3G^\circ$	3	124253	119944	102051	120529	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^3D^\circ$	2	124258	119958	102072	120545	—
$2s^22p^3(^2D^\circ_{3/2})3d$	$^1G^\circ$	4	124259	119952	102061	120538	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^3D^\circ$	1	124264	119959	102072	120546	—
$2s^22p^3(^2D^\circ_{5/2})3d$	$^1P^\circ$	1	124274	120043	103055	120030	—
$2s^22p^3(^2D^\circ_{3/2})3d$	$^1D^\circ$	2	124319	120017	102181	120609	—
$2s^22p^3(^2D^\circ_{3/2})3d$	$^1F^\circ$	3	124327	120033	102174	120629	—
$2s^22p^3(^2D^\circ_{3/2})3d$	$^3S^\circ$	1	124336	120002	102133	120577	—
$2s^22p^3(^2P^\circ)3d$	$^1D^\circ$	2	137928	137105	121625	141057	—
$2s^22p^3(^2P^\circ)3d$	$^3P^\circ$	0	137947	137093	121609	141050	—
$2s^22p^3(^2P^\circ)3d$	$^3P^\circ$	1	137947	137094	121611	141052	—
$2s^22p^3(^2P^\circ)3d$	$^3P^\circ$	2	137947	137097	121615	141054	—
$2s^22p^3(^2P^\circ)3d$	$^3D^\circ$	1	137963	137117	121642	141063	—
$2s^22p^3(^2P^\circ)3d$	$^3D^\circ$	2	137963	137119	121645	141066	—
$2s^22p^3(^2P^\circ)3d$	$^3D^\circ$	3	137963	137121	121647	141067	—
$2s^22p^3(^2P^\circ)3d$	$^1P^\circ$	1	137981	137186	121755	141153	—
$2s^22p^3(^2P^\circ)3d$	$^3F^\circ$	4	—	137084	121596	141041	—
$2s^22p^3(^2P^\circ)3d$	$^3F^\circ$	3	—	137085	121597	141041	—
$2s^22p^3(^2P^\circ)3d$	$^3F^\circ$	2	—	137085	121597	141041	—
$2s^22p^3(^2P^\circ)3d$	$^1F^\circ$	3	—	137136	121667	141098	—

3. Results and Discussion

3.1. Energy Levels.

We performed *ab initio* calculations of energy levels for O I using the three atomic structure codes CW, SS, and AS with the 5 configurations expansion $2p^4$, $2p^3\ 3s$, $2p^3\ 3p$, $2p^3\ 3d$, and $2p^3\ 4s$. This same set of configurations expansion was used by Tachiev and Froese Fischer (TFF) in the *ab initio* calculations [12] and by Froese Fischer and Tachiev in the *adjusted with experimental values* calculations [13]. For the SS and AS atomic codes, the scaling parameters are determined variationally by minimizing the sum of all the nonrelativistic term energies (Table 1).

In Tables 2–6, calculated fine structure energy levels are presented. The obtained values are compared with the NIST atomic database [22] and with Tachiev and Froese Fischer *ab initio* calculations [12] using the Multiconfiguration Hartree-Fock (MCHF) method [11].

For the fundamental configuration $2s^2\ 2p^4$, CW code gives 7% difference from NIST values, while SS and AS codes give, respectively, 15% and 19% difference from NIST values. With CW code and for the other four excited configurations ($2p^3\ 3\ell$, $\ell = 0, 1, 2$, and $2p^3\ 4s$), the agreement with NIST values is about 3%, while SS and AS give an agreement of about 20% with the NIST values except for $2p^3\ 3s$ where

Table 6: The same as Table 2 for configuration $2s^2$ $2p^3$ 4s.

Configuration	Term	J	E(NIST)	E(CW)	E(SS)	E(AS)	E(TFF)
$2s^2 2p^3(^4S^\circ)4s$	$^5S^\circ$	2	95477	92425	71070	110558	95576
$2s^2 2p^3(^4S^\circ)4s$	$^3S^\circ$	1	96225	93053	72757	122242	96264
$2s^2 2p^3(^2D^\circ)4s$	$^3D^\circ$	3	122420	118248	100741	144123	—
$2s^2 2p^3(^2D^\circ)4s$	$^3D^\circ$	2	122433	118247	100740	144121	—
$2s^2 2p^3(^2D^\circ)4s$	$^3D^\circ$	1	122441	118246	100739	144121	—
$2s^2 2p^3(^2D^\circ_{3/2})4s$	$^1D^\circ$	2	122798	118560	101552	149959	—
$2s^2 2p^3(^2P^\circ)4s$	$^3P^\circ$	0	*135682*	135369	120288	164620	—
$2s^2 2p^3(^2P^\circ)4s$	$^3P^\circ$	1	135682	135370	120289	164621	—
$2s^2 2p^3(^2P^\circ)4s$	$^3P^\circ$	2	135682	135372	120291	164623	—
$2s^2 2p^3(^2P^\circ)4s$	$^1P^\circ$	1	136353	135684	121113	170467	—

Table 7: Oscillator strengths for 3 multiplets $2p^4$-$2p^3(^4S)$ 3s $^3S^\circ$. g_i and g_k are, respectively, the statistical weights of initial and final levels of the transition. gf(NIST) are from NIST database [22]. gf(CW), gf(SS), and gf(AS) are calculated using, respectively, the Cowan, SUPERSTRUCTURE, and AUTOSTRUCTURE atomic codes. gf(FFT) are values from Froese Fisher and Tachiev [13] and gf(HBGV) are values from Hibbert et al. [6].

Terms	g_i	g_k	λ (Å)	gf(NIST)	gf(CW)	gf(SS)	gf(AS)	gf(FFT)	gf(HBGV)
^3P-$^3S^\circ$	1	3	1306.03	$5.19E-02$	$7.26E-02$	$1.39E-01$	$5.13E-02$	$4.78E-02$	$5.29E-02$
^3P-$^3S^\circ$	3	3	1304.86	$1.56E-01$	$2.18E-01$	$4.17E-01$	$1.54E-01$	$1.43E-01$	$1.59E-01$
^3P-$^3S^\circ$	5	3	1302.17	$2.60E-01$	$3.66E-01$	$6.95E-01$	$2.59E-01$	$2.40E-01$	$2.64E-01$
^1D-$^3S^\circ$	5	3	1641.31	$2.22E-06$	$6.04E-06$	$1.31E-05$	$6.95E-06$	$2.13E-06$	—
^1S-$^3S^\circ$	1	3	2324.74	$1.12E-08$	$3.08E-09$	$1.60E-08$	$5.50E-08$	$1.59E-10$	—

Table 8: The same as Table 7 for 4 multiplets $2p^3(^4S)3s$ S°-$2p^3(^4S)$ 3p P°.

Terms	g_i	g_k	λ (Å)	gf(NIST)	gf(CW)	gf(SS)	gf(AS)	gf(FFT)	gf(HBGV)
$^5S^\circ$-$^5P^\circ$	5	3	7775.39	$1.00E+00$	$1.09E+00$	$9.50E-01$	$2.00E+00$	$9.67E-01$	$1.01E+00$
$^5S^\circ$-$^5P^\circ$	5	5	7774.17	$1.67E+00$	$1.81E+00$	$1.58E+00$	$3.33E+00$	$1.61E+00$	$1.68E+00$
$^5S^\circ$-$^5P^\circ$	5	7	7771.94	$2.34E+00$	$2.54E+00$	$2.22E+00$	$4.67E+00$	$2.26E+00$	$2.35E+00$
$^5S^\circ$-$^3P^\circ$	5	3	6726.54	$1.31E-05$	$5.73E-07$	$9.21E-06$	$7.10E-05$	$1.02E-05$	—
$^5S^\circ$-$^3P^\circ$	5	5	6726.28	$4.00E-05$	$1.77E-06$	$2.81E-05$	$2.18E-04$	$3.51E-05$	—
$^3S^\circ$-$^5P^\circ$	3	3	10169.35	$9.16E-06$	$2.86E-06$	$1.68E-05$	$4.43E-05$	$7.91E-06$	—
$^3S^\circ$-$^5P^\circ$	3	5	10167.26	$2.80E-05$	$4.65E-08$	$5.51E-06$	$1.36E-04$	$2.74E-05$	—
$^3S^\circ$-$^3P^\circ$	3	1	8446.25	$3.44E-01$	$3.88E-01$	$3.81E-01$	$4.20E-01$	$3.39E-01$	$3.60E-01$
$^3S^\circ$-$^3P^\circ$	3	3	8446.76	$1.03E+00$	$1.16E+00$	$1.14E+00$	$1.26E+00$	$1.02E+00$	$1.08E+00$
$^3S^\circ$-$^3P^\circ$	3	5	8446.36	$1.72E+00$	$1.94E+00$	$1.91E+00$	$2.10E+00$	$1.70E+00$	$1.80E+00$

the agreement of AS with NIST is 4% and 7% for $2p^3$ 3d. AS gives bad energy levels (one hundred greater values) for the $2p^3$ 3p configuration comparing to the other data and the calculated values are not reported in Table 4. TFF energy levels are less than 1% near the NIST values but there are many missed values (they give energy levels for only 24% of the NIST data for the 4 excited configurations $2p^3$ $n\ell$).

We obtain six energy levels for the $2p^3$ 3p configuration ($2p^3(^2D^\circ)3p$ $^3P_{0,1,2}$ and $2p^3(^2P^\circ)3p$ $^3P_{0,1,2}$) and four new energy levels for the $2p^3$ 3d configuration ($2p^3(^2P^\circ)3d$ $^3F_{2,3,4}$ and $2p^3(^2P^\circ)3d$ $^1F_3$) which are not in the NIST atomic database (see the end of Tables 4 and 5).

3.2. Oscillator Strengths. We have also computed oscillator strengths for three multiplets of the transition $2p^4$-$2p^3$ 3s, four multiplets of the transition $2p^3$ 3s-$2p^3$ 3p, one multiplet of the transition $2p^4$-3d, and four multiplets of the transition $2p^3$ 3p-$2p^3$ 3d using the atomic structure codes CW, SS, and AS (see Tables 7–10). They are compared with those of FFT [13] and HBGV [6] and tabulated in NIST [22]. Our calculations with CW code give an agreement of about 2% with NIST values while FFT gives 8% with the NIST ones. The HBGV values have an agreement of 2% with the NIST ones but many data are missing.

4. Conclusions

The comparison between the energy levels calculated by the different atomic codes indicates that the agreement with NIST data is generally less than 20% except for the

TABLE 9: The same as Table 7 for the multiplet 2p^4 ^{3}P-2p^3(^{4}S) 3d ^{3}D$^\circ$.

Terms	g_i	g_k	λ (Å)	gf(NIST)	gf(CW)	gf(SS)	gf(AS)	gf(FFT)	gf(HBGV)
^{3}P- ^{3}D$^\circ$	5	7	1025.76	8.45E − 02	3.5E − 01	1.29E + 00	1.05E − 01	8.17E − 02	8.93E − 02
^{3}P-^{3}D$^\circ$	5	5	1025.76	1.51E − 02	6.24E − 02	2.31E − 01	1.87E − 02	1.46E − 02	1.59E − 02
^{3}P-^{3}D$^\circ$	5	3	1025.76	9.98E − 04	4.16E − 03	1.54E − 02	1.25E − 03	9.69E − 04	1.05E − 03
^{3}P-^{3}D$^\circ$	3	5	1027.43	4.52E − 02	1.87E − 01	6.94E − 01	5.60E − 02	4.37E − 02	4.10E − 02
^{3}P-^{3}D$^\circ$	3	3	1027.43	1.51E − 02	6.22E − 02	2.31E − 01	1.86E − 02	1.45E − 02	1.36E − 02
^{3}P-^{3}D$^\circ$	1	3	1028.16	2.00E − 02	8.30E − 02	3.09E − 01	2.48E − 02	1.94E − 02	2.12E − 02
^{3}P-^{5}D$^\circ$	5	7	1026.47*	—	8.45E − 09	1.00E − 06	5.79E − 09	4.35E − 07	—
^{3}P-^{5}D$^\circ$	5	5	1026.47*	—	1.13E − 07	3.25E − 06	4.36E − 08	3.65E − 08	—
^{3}P-^{5}D$^\circ$	5	3	1026.47*	—	6.64E − 08	1.60E − 06	3.87E − 08	7.14E − 09	—
^{3}P-^{5}D$^\circ$	3	5	1028.12*	—	1.32E − 08	1.76E − 08	3.66E − 08	1.10E − 07	—
^{3}P-^{5}D$^\circ$	3	3	1028.12*	—	4.48E − 08	1.33E − 06	—	1.07E − 07	—
^{3}P-^{5}D$^\circ$	1	3	1028.83*	—	3.85E − 08	5.62E − 07	—	1.44E − 07	—

*Wavelengths are from FFT.

TABLE 10: The same as Table 7 for 4 multiplets 2p^3(^{4}S) 3p P-2p^3(^{4}S) 3d D$^\circ$.

Terms	g_i	g_K	λ (Å)	gf(NIST)	gf(CW)	gf(SS)	gf(AS)	gf(FFT)	gf(HBGV)
^{5}P-^{3}D$^\circ$	5	7	9204.93	1.48E − 04	1.05E − 05	1.15E − 05	1.83E − 05	8.44E − 05	1.50E − 04
^{5}P-^{5}D$^\circ$	3	1	9260.81	5.74E − 01	6.73E − 01	5.42E − 01	1.08E − 01	5.90E − 01	6.75E − 01
^{5}P-^{5}D$^\circ$	3	3	9260.85	1.29E + 00	1.51E + 00	1.22E + 00	2.43E − 01	1.33E + 00	1.52E + 00
^{5}P-^{5}D$^\circ$	3	5	9260.94	1.00E + 00	1.18E + 00	9.49E − 01	1.89E − 01	1.03E + 00	1.18E + 00
^{5}P-^{5}D$^\circ$	5	3	9262.58	4.29E − 01	5.05E − 01	4.07E − 01	8.09E − 02	4.43E − 01	4.32E − 01
^{5}P-^{5}D$^\circ$	5	5	9262.67	1.67E + 00	1.96E + 00	1.58E + 00	3.15E − 01	1.72E + 00	1.68E + 00
^{5}P-^{5}D$^\circ$	5	7	9262.78	2.67E + 00	3.13E + 00	2.53E + 00	5.04E − 01	2.75E + 00	2.69E + 00
^{5}P-^{5}D$^\circ$	7	5	9265.83	1.91E − 01	2.24E − 01	1.81E − 01	3.60E − 02	1.97E − 01	1.92E − 01
^{5}P-^{5}D$^\circ$	7	7	9265.93	1.33E + 00	1.57E + 00	1.27E + 00	2.52E − 01	1.38E + 00	1.34E + 00
^{5}P-^{5}D$^\circ$	7	9	9266.01	5.15E + 00	6.05E + 00	4.88E + 00	9.73E − 01	5.31E + 00	5.19E + 00
^{3}P-^{3}D$^\circ$	3	5	11286.32	2.22E + 00	1.97E + 00	9.64E − 01	3.07E − 01	2.02E + 00	2.20E + 00
^{3}P-^{3}D$^\circ$	3	3	11286.41	7.40E − 01	6.58E − 01	3.22E − 01	1.02E − 01	6.74E − 01	7.32E − 01
^{3}P-^{3}D$^\circ$	5	7	11286.91	4.13E + 00	3.68E + 00	1.80E + 00	5.71E − 01	3.77E + 00	4.10E + 00
^{3}P-^{3}D$^\circ$	5	5	11287.03	7.40E − 01	6.56E − 01	3.22E − 01	1.02E − 01	6.74E − 01	7.32E − 01
^{3}P-^{3}D$^\circ$	5	3	11287.12	4.93E − 02	4.38E − 02	2.14E − 02	6.80E − 03	4.49E − 02	4.88E − 02
^{3}P-^{3}D$^\circ$	1	3	11287.32	9.86E − 01	8.77E − 01	4.28E − 01	1.37E − 01	8.98E − 01	9.76E − 01
^{3}P-^{5}D$^\circ$	1	3	11373.92	2.32E − 05	1.11E − 06	8.55E − 07	3.56E − 07	1.43E − 05	2.00E − 05
^{3}P-^{5}D$^\circ$	5	7	11374.01	1.37E − 04	1.32E − 06	6.93E − 07	1.44E − 05	5.16E − 04	1.50E − 04

configuration 2p^3 3p where the SS gives 20% greater values than NIST and CW gives only 3% greater values than NIST.

We obtained, respectively, six and four energy levels corresponding to the configurations 2p^3 3p and 2p^3 3d which are not in the NIST atomic database.

TFF energy levels values are nearly the same compared to NIST ones with less than 1% difference but many energy levels are missed in these calculations.

When comparing oscillator strengths calculated by AS code, we obtain good agreement with NIST.

We can say that there is no best atomic code to use and we have to calculate atomic structure data with more than one code to compare results between them and with other theoretical and experimental sources.

Competing Interests

The authors declare that there are no competing interests regarding the publication of this paper.

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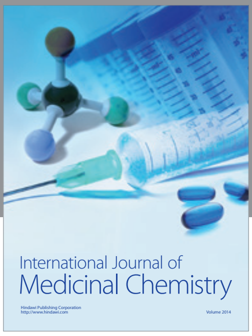
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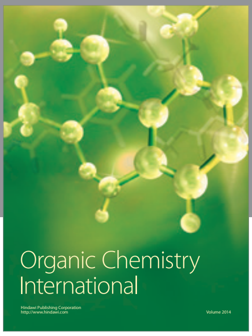
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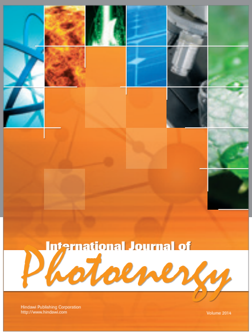
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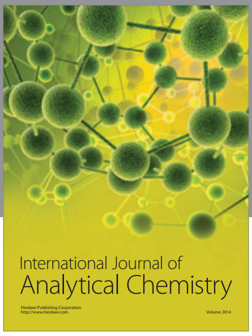
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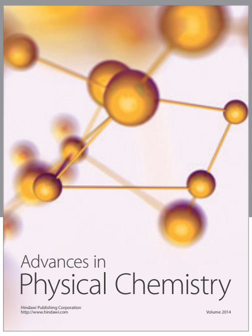
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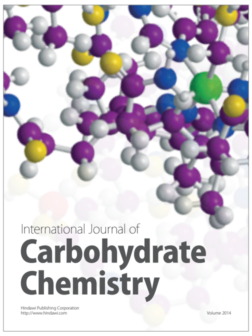
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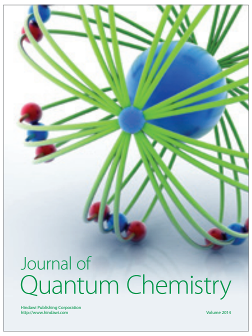
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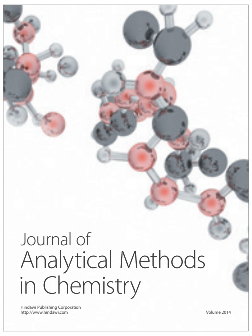
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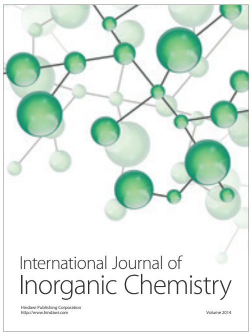
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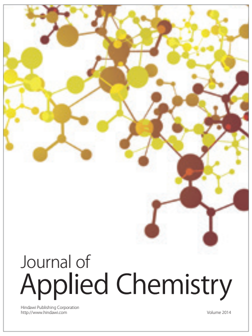
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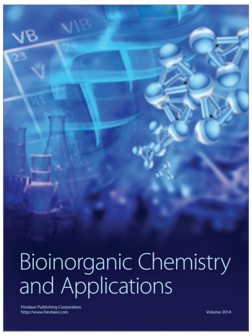
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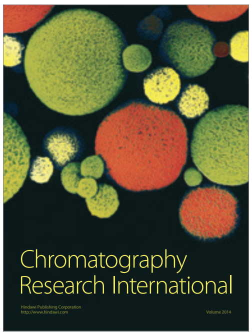
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