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ACCURATE CALCULATIONS OF INTERSTELLAR LINES OF Mg^+ USING THE COUPLED CLUSTER APPROACH

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ABSTRACT

One of the most successful ab initio, highly correlated all-order many-body methods, the relativistic coupled cluster theory, is employed to calculate excitation energies of the doublet states of Mg^+ and allowed transitions among them that are of interest in astrophysical problems. We have also calculated oscillator strength for the $3s$–$4p$ doublet transitions, which is improved over the existing results. These transition lines have been sought after in astronomical observations because they represent the best column density identifier in the interstellar medium. Our calculated oscillator strength (9.3×10^{-4}) and branching ratio (1.80) of these doublet lines matches well with the recent empirical and semiempirical calculations.

Subject headings: atomic data — methods: analytical

1. INTRODUCTION

Atoms and ions with single-valence electrons play an important role in a variety of astrophysical situations. Earlier works on the oscillator strength of the transitions from the valence electrons of these atomic systems had been focused primarily on the strong $ns \rightarrow np$ transitions. The intensity of successive lines $ns \rightarrow n'p$ decreases rapidly with increasing n'. Systematic calculations have shown this behavior of alkali spectra to be only one example of a general feature of absorption spectra due to the nonhydrogenic character of realistic potentials $V(r)$ (Fano & Cooper 1968).

The combination of high spectral resolution, photometric precision, and sensitivity provided by many recent spectrographs has motivated the study of UV interstellar absorption lines. This study enables a detailed examination of individual absorption regions in the interstellar medium (ISM). The strong near-UV Mg II lines are generally highly saturated along most interstellar lines outside the local ISM and usually yield extremely uncertain estimates of Mg II column densities in interstellar gas. Since Mg^+ is the dominant form of Mg in the neutral ISM, i.e, H I gas, and since Mg is expected to be a significant constituent of interstellar dust grains, the far-UV lines are critical for assessing the role of this important element in the ISM. Along most of the interstellar lines—with the exception of those that pass only through the local ISM (Linsky & Wood 1996)—the near-UV Mg II $\lambda\lambda$2796, 2803 lines are strongly saturated and yield limited column density information. The neutral source of accurate Mg II column densities is thus the other pair of observationally accessible Mg II lines, the intrinsically much weaker doublets around λ1240 discussed below.

Magnesium is one of the most abundant metals in the interstellar dust, as it readily condenses into solid form. In addition, Mg provides a diagnostic of electron density in the gas phase of the ISM, through the ionization ratio Mg/Mg^+. An accurate assessment of the importance of Mg in both the gas and the dust must clearly start with accurate column densities.

In addition to the two strong lines of Mg^+, $3s\,S_{1/2} \rightarrow 4p\,P_{1/2,3/2}$ transitions have been observed in the ultraviolet region at approximately 1240 Å. As mentioned earlier, this doublet transition is very weak. The empirical oscillator strength value calculated by Morton & Hu (1975) is 2.6 times larger than the theoretical value provided by Black, Weisheit, & Laviana (1972) for this transition. However, the oscillator strength calculated later using various methods yields smaller values than expected.

In recent years, many ab initio semiempirical and empirical calculations have been performed (Hibbert et al. 1983; Fitzpatrick 1997; Fleming et al. 1998; Theodosiou & Federman 1999; Sofia, Fabian, & Howk 2001). There are discrepancies between the empirical f-values of Mg II $\lambda\lambda$1239, 1240 lines obtained from the absorption toward the astronomical objects (Fitzpatrick 1997; Sofia et al. 2001) and ab initio calculations performed by Hibbert et al. (1983). The improved ab initio calculations by Fleming et al. (1998) are not in very good agreement with the recent empirical calculations by Fitzpatrick (1997) and Sofia et al. (2001) and semiempirical calculations by Theodosiou & Federman (1999). We employ the ab initio relativistic all-order many-body coupled cluster (CC) method with single, double, and partial triple excitations (CCSD[T]) to calculate allowed transitions of Mg II. We compare our calculations with results obtained by empirical and semiempirical calculations for the weak doublets and also the all-order relativistic single-double (SD) method (Safronova, Derevianko, & Johnson 1998) for the resonance line.

2. THEORY

In the relativistic CC approach, one first considers the relativistic Hartree-Fock (also known as the Dirac-Fock [DF]) reference state corresponding to an $N-1$ electron closed-shell configuration, then adds one electron to the $k^{\rm th}$ virtual orbital and obtains the N electron system on which calculations are carried out. The addition of an electron to the $k^{\rm th}$

virtual orbital to the reference state can therefore be written as

$$|\Phi_k^N\rangle = a_k^+|\Phi_0\rangle \ .$$

Any general state can be written in the open-shell CC method (Lindgren & Morrison 1985) as

$$|\Psi_k\rangle = e^T\{e^{S_k}\}|\Phi_k\rangle \ ,$$

where $|\Phi_k\rangle$ is the DF reference state for an open-shell configuration with T and S operators defined as

$$T = T_1 + T_2 = \sum_{ap} a_p^+ a_a t_a^p + \sum_{abpq} a_p^+ a_q^+ a_b a_a t_{ab}^{pq} \ ,$$

$$S_k = S_{k1} + S_{k2} = \sum_{p} a_p^+ a_k s_k^p + \sum_{pqa} a_p^+ a_q^+ a_a a_k s_{ka}^{pq} \ .$$

Here T represents the operator that produces excitations from the core and S the excitation from valence and valence-core interactions. In our notation, a, b,... denote core orbitals, and p, q, r,... denote virtual orbitals.

The T and S operators introduce correlations induced by interactions among electrons. Because of these interactions, there are multiple powers of single (T_1, S_1) and double (T_2, S_2) excitations from the reference states $|\Phi_k\rangle$, which are part of higher excitations. By the principle of linear superposition of wave functions, all the configurations obtained from these excitations will contribute to the exact state $|\Psi_k\rangle$, with the proviso that we must include a statistical weighting factor to avoid counting them more than once. The sum of all the multiple powers of the particular excitation operator (say, T_i, $i = 1$ or 2) with the weighting factors gives rise to the exponential character of it (e^{T_i}), which will have a form of e^T when we consider all the terms containing T_1 and T_2. In a similar way, the e^S operator is introduced in the $|\Psi_k\rangle$ expression.

We solve the Dirac-Coulomb equation given by

$$H|\Psi^{N-1}\rangle = E^{N-1}|\Psi^{N-1}\rangle \ , \tag{1}$$

where $H = \sum_i c\alpha_i \cdot \boldsymbol{p}_i + (\beta_i - 1)c^2 + V_N + \sum_{i<j}(1/r_{ij})$.

By suitable substitutions, using the T operator we obtain two equations. One of them gives the CC amplitudes

$$\langle\Phi'|\bar{H}_N|\Phi_0\rangle = 0 \tag{2}$$

and the correlation energy of the $N-1$ electron system

$$\langle\Phi_0|\bar{H}_N|\Phi_0\rangle = \Delta E^{N-1} \ , \tag{3}$$

where $\langle\Phi'|$ is singly or doubly excited configurations from the $\langle\Phi_0|$, and $H_N = H - \langle\Phi_0|H|\Phi_0\rangle$ and $\bar{H}_N = e^{-T}H_N e^T$.

The Schrodinger equation, which we solve here, is given by

$$H|\Psi_k^N\rangle = E_k^N|\Psi_k^N\rangle \ . \tag{4}$$

Carrying out mathematical operations similiar to those used earlier involving the T and S operators, we obtain an equation for the ionization potential (IP) and another one for the CC amplitudes (Gopakumar et al. 2001). The equation for the evaluation of the ionization potential is

$$\langle\Phi_k^N|\bar{H}_N(1 + S_k)|\Phi_k^N\rangle = \Delta E_k^N \ , \tag{5}$$

and the equation for the CC amplitudes is

$$\langle\Phi_k^{*,N}|\bar{H}_N S_k|\Phi_k^N\rangle = \Delta E_k^N\langle\Phi_k^{*,N}|S_k|\Phi_k^N\rangle - \langle\Phi_k^{*,N}|\bar{H}_N|\Phi_k^N\rangle \ . \tag{6}$$

Here we first solve for ΔE_k^N using equation (5), and then solve equation (6) to get new S amplitudes, which we use in turn to get new ΔE_k^N until self-consistency is achieved. Excitation energy from the $k^{\rm th}$ orbital to the $l^{\rm th}$ orbital will be the difference of IP between the $k^{\rm th}$ and $l^{\rm th}$ orbitals.

Triple excitations are included in an approximate way (Bartlett 1995; Chaudhuri, Mukhopadhyay, & Mukherjee 1989). This contribution is added to the energy obtained using singles and doubles.

The definition of the oscillator strength of a transition from $|\Psi_i\rangle$ to $|\Psi_f\rangle$ is

$$f_L = \frac{2}{3g_i}\Delta E_{fi}|D_{fi}|^2 \ , \tag{7}$$

where ΔE_{fi} is the energy difference between final state and initial state, g_i is the degeneracy factor of the initial state, and the electric dipole moment matrix element D_{fi} is defined as

$$D_{fi} = \frac{\langle\Psi_f|\boldsymbol{d}|\Psi_i\rangle}{\sqrt{\langle\Psi_f|\Psi_f\rangle}\sqrt{\langle\Psi_i|\Psi_i\rangle}} \ , \tag{8}$$

where

$$\langle\Psi_f|\boldsymbol{d}|\Psi_i\rangle = \langle\Phi_f^{n+1}|\{e^{S_f^{aa}}\}\bar{\boldsymbol{d}}\{e^{S_i}\}|\Phi_i^{n+1}\rangle \ , \tag{9}$$

$\bar{\boldsymbol{d}} = e^{-T}\boldsymbol{d}e^T$, and d is the electric dipole moment operator in length form. The connected parts of equations (6) and (7) will contribute, and hence we only compute those parts in our dipole matrix element calculations.

3. RESULTS AND DISCUSSION

The DF reference state of Mg^+ was calculated using a new approach (Majumder et al. 2001). Our calculated ionization potential of the $3s$ orbital is 121117.91 cm^{-1}, which differs from the experimental value by 0.12%. In Table 1, we present the excitation energies of the doublet states calculated using the CCSD(T) and compare them with the National Institute of Standards and Technology (NIST) data[1] and values obtained from other calculations (Hibbert et al. 1983; Fleming et al. 1998; Safronova et al. 1998). The accuracy of the results obtained using the all-order relativistic SD method (Safronova et al. 1998) are comparable with the CCSD(T) results. Safronova et al. (1998) have shown that the effect of Breit interaction is almost negligible. Some moderate and large configuration interaction (CI) calculations were performed by Hibbert et al. (1983) and Fleming et al. (1998), respectively, to calculate the excitation energies. However, the results of those calculations do not agree as well with the NIST data, which are compiled from experimental measurements, as our CCSD(T) calculations. This highlights the advantages of the CC method over the CI approach, as discussed by Bartlett (1995). In Table 1, we present the energies of low-lying bound states of different symmetries.

[1] See http://aeldata.phy.nist.gov/nist_beta.html.

TABLE 1

EXCITATION ENERGIES FROM THE GROUND STATE IN cm^{-1}

States	Multiplet	NIST[a]	CCSD(T)[b]	Others
$2p^6 3p$.....	$^2P_{1/2}$	35669.31	35652.26	35489.04,[c] 35730.47,[d] 35663.5[e]
	$^2P_{3/2}$	35760.88	35746.01	35754.8[e]
$2p^6 4s$	$^2S_{1/2}$	69804.95	69723.49	68827.24,[c] 69804.4[e]
$2p^6 3d$.....	$^2D_{3/2}$	71491.06	71404.68	71494.8[e]
	$^2D_{5/2}$	71490.19	71404.21	71493.9[e]
$2p^6 4p$.....	$^2P_{1/2}$	80619.50	80534.64	79581.50,[c] 80174.08[d]
	$^2P_{3/2}$	80650.02	80565.83	...
$2p^6 5s$	$^2S_{1/2}$	92790.51	92688.34	91542.87[c]
$2p^6 4d$.....	$^2D_{3/2}$	93311.11	93208.29	...
	$^2D_{5/2}$	93310.59	93207.96	...
$2p^6 4f$	$^2F_{5/2}$	93799.63	93681.63	...
	$^2D_{7/2}$	93899.75	93681.76	...
$2p^6 5p$.....	$^2P_{1/2}$	97455.12	97352.16	96195.73[c]
	$^2P_{3/2}$	97468.92	97366.30	...
$2p^6 6s$	$^2S_{1/2}$	103196.75	103108.93	101858.17[a]
$2p^6 5d$.....	$^2D_{3/2}$	103420.00	103309.98	...
	$^2D_{5/2}$	103419.70	103309.79	...
$2p^6 5f$	$^2F_{5/2}$	103689.86	103570.15	...
	$^2D_{7/2}$	103689.92	103570.21	...
$2p^6 6p$.....	$^2P_{1/2}$	105622.34	105516.19	...
	$^2P_{3/2}$	105629.72	105523.95	...

[a] Reference of http://aeldata.phy.nist.gov/nist_beta.html.
[b] Work presented in this paper.
[c] CI method (Hibbert et al. 1983).
[d] Superposition of configuration method (Fleming et al. 1998).
[e] Relativistic SD method (Safronova et al. 1998).

An important motivation of this work is to calculate $3s$–$4p$ transitions to high accuracy. Fano & Cooper (1968) have argued that this transition amplitude should be small. That is due to cancellations of the positive and negative contributions to the radial integrals (Fano & Cooper 1968). Fleming et al. (1998) have recently carried out a large-scale nonrelativistic CI calculation for this transition. They obtained an oscillator strength of 8.33×10^{-4}, which is higher than the value found in earlier CI calculations (3.7×10^{-4}) (Hibbert et al. 1983). In our calculation, we have achieved an accurate description of electron correlation by taking all the single, double, and partial triple excitations of all the electrons from the core into a large virtual space. Our results agree very well with all the empirical (Fitzpatrick 1997; Sofia et al. 2001) and semiempirical (Theodosiou & Federman 1999) results. This is shown in Table 2, along with a comparison of the branching ratio (BR) of these weak doublets. Our calculated BR confirms all the empirical and semiempirical calculations that the BR should be less than 2. Sofia et al. (2001) have shown the importance of this result in their calculations.

We have calculated velocity-gauge electric dipole matrix elements for all the transitions presented in Table 4. A comparison of these matrix elements with the corresponding matrix elements calculated using length gauge is presented in Table 3 for a few transitions. Comparison shows good agreement between the results calculated from the two gauges, even though it is not easy to achieve, and it indicates the accuracy of the calculations. The small disagreement may be improved by using experimental transition energies and including larger basis.

In Table 4, we give the oscillator strengths (using length gauge) of all the possible doublet allowed transitions, *ms*–*np*, *mp*–*nd*, and *md*–*nf*, for various *m* and *n* calculated using the CCSD(T) method. A comparison is made with the NIST data and the all-order relativistic many-body perturbation theory (MBPT) calculations (Safronova et al. 1998). The all-order MBPT calculations performed by Safronova et al. are based on the inclusion of single and double excitations from the DF reference state, and it is referred to by the authors as the relativistic SD method. They have calculated a few strong transitions using this approach. Their calcu-

TABLE 2

OSCILLATOR STRENGTHS (OF THE ORDER OF 10^{-4}) AND BRANCHING RATIO (BR) OF A $3s$–$4p$ TRANSITION

Transitions	Multiplets	Fitzpatrick (1997)	Theodosiou & Federman (1999)	Theodosiou & Federman (1999)	Sofia et al. (2001)	CI[a]	CCSD(T)[b]
$3s$–$4p$.....	$^2S_{1/2}$–$^2P_{1/2}$	3.2 ± 0.2	3.37 ± 0.21	3.56 ± 0.05	3.54 ± 0.12	2.77	3.322
	$^2S_{1/2}$–$^2P_{3/2}$	6.4 ± 0.4	6.13 ± 0.39	6.32 ± 0.05	6.17 ± 0.2	5.53	5.980
BR	...	2	1.82 ± 0.08	1.78 ± 0.03	1.74 ± 0.06	2	1.8

[a] See Fleming et al. 1998.
[b] Work presented in this paper.

TABLE 3
Comparison between the Transition Matrix Elements Calculated Using Length and Velocity Gauges

Transitions	Multiplets	Length Gauge	Velocity Gauge
$3s$–$3p$.....	$^2S_{1/2}$–$^2P_{1/2}$	2.368	2.275
$3s$–$4p$.....	$^2S_{1/2}$–$^2P_{1/2}$	0.052	0.056
$4s$–$4p$.....	$^2S_{1/2}$–$^2P_{1/2}$	5.346	5.205
$3p$–$3d$	$^2P_{1/2}$–$^2D_{3/2}$	4.147	3.917

lated oscillator strengths (f-value) are in good agreement with our present work. We have calculated many transitions for which no values could be found in the literature. Almost all the values obtained from the NIST database shown here are compiled from the earlier nonrelativistic semiempirical calculations or relativistic Hartree-Fock–type calculations (references are available on-line).[1] There are small differences between the available f-values obtained from the NIST database and our calculations using the CCSD(T) method apart from the weak $S \rightarrow P$ weak transitions.

TABLE 4
Oscillator Strengths of Various Transitions

Transitions	Multiplets	NIST[a]	CCSD[b]	MCDF[c]	Relative SD[d]
$3s$–$3p$.....	$^2S_{1/2}$–$^2P_{1/2}$	0.306	0.30365	0.30320	0.30403
	$^2S_{1/2}$–$^2P_{3/2}$	0.609	0.60899	0.60952	0.60989
$3s$–$4p$.....	$^2S_{1/2}$–$^2P_{1/2}$	7.7E−5	3.322E−4	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	1.5E−4	5.980E−4	...	...
$3s$–$5p$.....	$^2S_{1/2}$–$^2P_{1/2}$	3.3E−3	3.921E−4	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	6.6E−3	7.427E−4	...	...
$3s$–$6p$.....	$^2S_{1/2}$–$^2P_{1/2}$	...	7.593E−6	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	...	1.953E−5	...	...
$3p$–$4s$.....	$^2P_{1/2}$–$^2S_{1/2}$	0.138	0.14561	0.1533	0.14427
	$^2P_{3/2}$–$^2S_{1/2}$	0.139	0.14563	0.1595	0.14943
$3p$–$5s$.....	$^2P_{1/2}$–$^2S_{1/2}$	...	0.01763	...	...
	$^2P_{3/2}$–$^2S_{1/2}$	...	0.01767	...	...
$3p$–$6s$.....	$^2P_{1/2}$–$^2S_{1/2}$	...	6.027E−3	...	...
	$^2P_{3/2}$–$^2S_{1/2}$	...	6.066E−3	...	...
$3p$–$3d$	$^2P_{1/2}$–$^2D_{3/2}$	0.920	0.93669	...	0.94086
	$^2P_{3/2}$–$^2D_{3/2}$	0.0919	0.09358	...	0.09409
	$^2P_{3/2}$–$^2D_{5/2}$	0.828	0.84226	...	0.84716
$3p$–$4d$	$^2P_{1/2}$–$^2D_{3/2}$	...	3.8462E−2	...	...
	$^2P_{3/2}$–$^2D_{3/2}$	...	3.844E−3	...	...
	$^2P_{3/2}$–$^2D_{5/2}$	...	3.8463E−2	...	...
$3p$–$5d$	$^2P_{1/2}$–$^2D_{3/2}$	...	1.236E−2	...	...
	$^2P_{3/2}$–$^2D_{3/2}$	...	1.265E−3	...	...
	$^2P_{3/2}$–$^2D_{5/2}$	...	1.139E−2	...	...
$3d$–$4p$	$^2D_{3/2}$–$^2P_{1/2}$	0.149	0.15131	...	...
	$^2D_{3/2}$–$^2P_{3/2}$	0.029	0.03034	...	...
	$^2D_{5/2}$–$^2P_{3/2}$	0.178	0.18105	...	...
$3d$–$5p$	$^2D_{3/2}$–$^2P_{1/2}$	0.0039	3.886E−3	...	...
	$^2D_{3/2}$–$^2P_{3/2}$	7.8E−4	7.814E−4	...	...
	$^2D_{5/2}$–$^2P_{3/2}$	0.0047	4.659E−3	...	...
$3d$–$4f$.....	$^2D_{3/2}$–$^2F_{5/2}$	0.95	0.97246	...	...
	$^2D_{5/2}$–$^2F_{5/2}$	...	0.04605	...	...
	$^2D_{5/2}$–$^2F_{7/2}$	...	0.92115	...	...
$3d$–$5f$.....	$^2D_{3/2}$–$^2F_{5/2}$	0.164	0.15926	...	...
	$^2D_{5/2}$–$^2F_{5/2}$	...	7.542E−3	...	...
	$^2D_{5/2}$–$^2F_{7/2}$	...	0.15085	...	...
$4s$–$4p$.....	$^2S_{1/2}$–$^2P_{1/2}$	0.456	0.46478	0.442	...
	$^2S_{1/2}$–$^2P_{3/2}$	0.91	0.93224	0.843	...
$4s$–$5p$.....	$^2S_{1/2}$–$^2P_{1/2}$	3.4E−4	8.366E−4	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	6.9E−4	1.745E−3	...	...
$4s$–$6p$.....	$^2S_{1/2}$–$^2P_{1/2}$	...	9.922E−5	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	...	2.237E−4	...	...
$4p$–$4d$	$^2P_{1/2}$–$^2D_{3/2}$	1.23	1.22868	...	...
	$^2P_{3/2}$–$^2D_{3/2}$	0.124	0.12285	...	...
	$^2P_{3/2}$–$^2D_{5/2}$	1.11	1.10562	...	...
$4p$–$5s$.....	$^2P_{1/2}$–$^2S_{1/2}$	0.263	0.26105	...	...
	$^2P_{3/2}$–$^2S_{1/2}$	0.264	0.26108	...	...
$4p$–$6s$.....	$^2P_{1/2}$–$^2S_{1/2}$	0.0315	0.02987	...	...
	$^2P_{3/2}$–$^2S_{1/2}$	0.0315	0.03002	...	...
$4p$–$5d$	$^2P_{1/2}$–$^2D_{3/2}$	0.083	0.09699	...	...
	$^2P_{3/2}$–$^2D_{3/2}$	0.005	9.743E−3	...	...
	$^2P_{3/2}$–$^2D_{5/2}$	0.074	0.08772	...	...

TABLE 4—*Continued*

Transitions	Multiplets	NIST[a]	CCSD[b]	MCDF[c]	Relative SD[d]
4*d*–4*f*	$^2D_{3/2}$–$^2F_{5/2}$	...	0.05596	...	...
	$^2D_{5/2}$–$^2F_{5/2}$	...	2.654E−3	...	...
	$^2D_{5/2}$–$^2F_{7/2}$	...	0.05309	...	...
4*d*–5*p*	$^2D_{3/2}$–$^2P_{1/2}$	...	0.30105	...	...
	$^2D_{3/2}$–$^2P_{3/2}$	...	0.06029	...	...
	$^2D_{5/2}$–$^2P_{3/2}$	...	0.36001	...	...
4*d*–6*p*	$^2D_{3/2}$–$^2P_{1/2}$	...	...	...	...
	$^2D_{3/2}$–$^2P_{3/2}$	...	...	...	...
	$^2D_{5/2}$–$^2P_{3/2}$	...	...	...	...
4*d*–5*f*	$^2D_{3/2}$–$^2F_{5/2}$	0.80	0.79765	...	...
	$^2D_{5/2}$–$^2F_{5/2}$	...	3.7782E−2	...	...
	$^2D_{5/2}$–$^2F_{7/2}$	...	0.75569	...	...
5*s*–5*p*	$^2S_{1/2}$–$^2P_{1/2}$	...	0.61204	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	...	1.22678	...	...
5*s*–6*p*	$^2S_{1/2}$–$^2P_{1/2}$	...	2.771E−3	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	...	5.789E−3	...	...
5*p*–6*s*	$^2P_{1/2}$–$^2S_{1/2}$	...	0.37715	...	...
	$^2P_{3/2}$–$^2S_{1/2}$	...	0.37964	...	...
5*p*–5*d*	$^2P_{1/2}$–$^2D_{3/2}$	...	1.88856	...	...
	$^2P_{3/2}$–$^2D_{3/2}$	...	0.19083	...	...
	$^2P_{3/2}$–$^2D_{5/2}$	...	1.71708	...	...
5*d*–6*p*	$^2D_{3/2}$–$^2P_{1/2}$	...	...	...	...
	$^2D_{3/2}$–$^2P_{3/2}$	...	...	...	...
	$^2D_{5/2}$–$^2P_{3/2}$	...	...	...	...
5*d*–5*f*	$^2D_{3/2}$–$^2F_{5/2}$	...	0.11006	...	...
	$^2D_{5/2}$–$^2F_{5/2}$	...	5.416E−3	...	...
	$^2D_{5/2}$–$^2F_{7/2}$	...	0.10834	...	...
6*s*–6*p*	$^2S_{1/2}$–$^2P_{1/2}$	...	0.76690	...	...
	$^2S_{1/2}$–$^2P_{3/2}$	...	1.53734	...	...

[a] See http://aeldata.phy.nist.gov/nist_beta.html.
[b] CCSD work presented here.
[c] We have done Multiconfiguration Dirac-Fock calculations for some possible transitions to cross-check our results.
[d] Safronova et al. 1998.

4. CONCLUSION

This work focuses on the oscillator strengths and BR for 3*s*–4*p* transition, as well as all allowed bound-bound transitions among the doublet states. This is the first fully ab initio calculation in which both the parameters agree very well with recent empirical and semiempirical calculations. Our BR calculations confirm the claim of Sofia et al. (2001) that it should be less than 2, which is very important because of the high quality of spectra. Our calculated excitation energies are of high accuracy and agree within 0.1% with the NIST values. There is excellent agreement of our calculated oscillator strengths using the CCSD(T) method with those obtained using the relativistic SD method wherever available. Among the important features of our CCSD(T) calculations is the inclusion of nonlinear singles, doubles, and partial triples cluster amplitudes in the wave functions, leading to more accurate and reliable results.

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