

Article



Radiative Properties of Rb-Isoelectronic Technetium (Tc VII), Ruthenium (Ru VIII) and Rhodium (Rh IX) Ions for Astrophysical Applications

Jyoti ^{1,*}, Mandeep Kaur ¹ and Bindiya Arora ^{1,2}

- ¹ Department of Physics, Guru Nanak Dev University, Amritsar 143005, Punjab, India
- ² Perimeter Institute for Theoretical Physics, Waterloo, ON N2L 2Y5, Canada
- * Correspondence: arora.jyoti326@gmail.com or jyotiphy.rsh@gndu.ac.in

Abstract: In this work, we present high-accuracy spectroscopic properties, such as line strengths, transition probabilities and oscillator strengths for allowed transitions among $nD_{3/2,5/2}$, $n'S_{1/2}$ and $n'P_{1/2,3/2}$ (n = 4, n' = 5, 6) states of Rb-isoelectronic Tc (Tc VII), Ru (Ru VIII) and Rh (Rh IX) ions for their applications in the analysis of astrophysical phenomena occurring inside celestial bodies containing Tc, Ru and Rh ions. Due to the scarcity of computational data of atomic properties of these transitions, as well as considerable discrepancies within the literature about these ions, the precise determination of these properties is necessary. For this purpose, we have implemented relativistic many-body perturbation theory (RMBPT) for evaluation of the wave functions of the considered states. For better accuracy, we have accounted for electron interactions through random phase approximation, Brückner orbitals and structural radiations of wave functions in our RMBPT method for further precise evaluation of electric dipole amplitudes. Combining these values of the observed wavelengths, the above transition properties and radiative lifetimes, a number of excited states of Tc VII, Ru VIII and Rh IX ions have been calculated. For further validation of our work, we have compared our results with the data already available in the literature.

Keywords: relativistic many body perturbation theory; line strength; transition probability; oscillator strength; radiative lifetime

1. Introduction

With pioneering innovations in science and technology, the study of atmosphere, chemical abundances and the evolution of stars has recently been of interest. Nowadays, numerous investigations have been carried out to detect the presence of various elements and ions in different celestial bodies. The spectral analysis of different celestial objects has revealed the presence of highly charged ions in their environments, of which technetium (Tc), ruthenium (Ru) and rhodium (Rh) ions are of particular interest to us. Technetium is an s-process element with no stable isotope, whereas ruthenium and rhodium are classified as the refractory components of cosmological objects [1]. The absorption of spectral lines of Tc was first identified in the spectra of several S and M stars by Merrill [2]. The presence of Tc in the atmosphere of red giant stars reflects the occurrence of s-process nucleosynthesis in evolved stars. Tc spectral lines were observed in the high-resolution HERMES spectra of BD+79°156 [3]. Moreover, the instability of Tc depicts the decay of Tc into Ru through s-process, indicating the possible presence of Ru in Tc-rich stars. Furthermore, considerable abundance of the platinum group elements, including Ru and Rh have recently been analyzed by Fischer–Gödde et al. [1] in chondritic meteorites, which elevates the importance of studying the radiative properties of these elements and ions.

The knowledge of precise radiative properties is important for stellar analysis [4] and to infer the mass (M), radius (R) and luminosity (L) of stars [5,6]. These radiative properties are also useful in the analysis of interstellar and quasar absorption of lines, as well as the



Citation: Jyoti; Kaur, M.; Arora, B. Radiative Properties of Rb-Isoelectronic Technetium (Tc VII), Ruthenium (Ru VIII) and Rhodium (Rh IX) Ions for Astrophysical Applications. *Atoms* 2022, *10*, 138. https://doi.org/10.3390/ atoms10040138

Academic Editors: Izumi Murakami, Daiji Kato, Hiroyuki A. Sakaue and Hajime Tanuma

Received: 5 September 2022 Accepted: 9 November 2022 Published: 11 November 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). photospheric abundance of the considered element in a given star [7]. The construction of kinetic models of plasma processes and the experimental investigations in thermonuclear reactor plasma [8,9], the estimation of the electron collisional rate coefficients and photoionization cross-sections for various scattering phenomena [10–12], and the assessment of Stark broadening of spectral lines involving different astrophysical phenomena [13], also aspire to more precise estimation of these radiative properties.

A limited number of studies involving the properties of Rb-isoelectronic Tc, Ru and Rh ions have been reported thus far. Until now, Das et al. [14] and Migdalek [15] determined the spectroscopic properties of Tc VII, whereas Zilitis [16] considered these ions for the evaluation of oscillator strengths at Dirac-Fock level. Unfortunately, we did not find any other literature providing the relativistic spectroscopic data of the ions under consideration here.

The presence of Tc, Ru and Rh ions in giant stars, chondritic meteorites and solar abundances motivated us to determine the radiative properties of these ions. Moreover, the scarcity of radiative data in the available theoretical literature led us to extend our study to determine these radiative properties among $nD_{3/2,5/2}$, $n'S_{1/2}$ and $n'P_{1/2,3/2}$ (n = 4, n' = 5, 6) states, along with the evaluation of radiative lifetimes of $5P_{1/2,3/2}$ and $6S_{1/2}$ states of the ions we studied. We have also calculated ionization energies of different states involved in our transitions in this work. The validation of our study was carried out by conducting a comparison of our results with available theoretical data wherever possible.

2. Theoretical Aspects and Formulae Used

Different spectroscopic properties of Rb-isoelectronic ions were analyzed through the E1 decay channel, as electrons in the considered systems decay from excited states dominantly through the allowed transitions. The transition probability of the E1 decay channel (A_{vk}^{E1}) for the transition between the lower state $|\psi_k\rangle$ and the upper state $|\psi_v\rangle$, with corresponding angular momenta J_k and J_v , is given by [17,18]

$$A_{vk}^{E1} = \frac{2}{3}\alpha c\pi\sigma \times \left(\frac{\alpha\sigma}{R_{\infty}}\right)^2 \frac{S^{E1}}{g_v} = A_{vk}^{E1} = \frac{2.02613 \times 10^{18}}{g_v \lambda^3} S^{E1},\tag{1}$$

where $\alpha = \frac{e^2}{2\epsilon_0 hc}$ is the fine structure constant, c is the speed of light and σ denotes the differential energy between the transition levels given by $\sigma = E_v - E_k$. Here, λ and S are used in Å and a.u., respectively, and $g_v = 2J_v + 1$ depicts the degeneracy factor for the corresponding state $|\psi_v\rangle$, R_∞ is the Rydberg constant and S^{E1} denotes the line strength, which is actually the square of the reduced E1 matrix element of the considered transition. Numerically, the line strength of the transition occurring between the states $|\psi_k\rangle$ and $\psi_v\rangle$ can be given by $S^{E1} = |\langle \psi_v | | \mathbf{D} | | \psi_k \rangle|^2$ [19] with $\mathbf{D} = \Sigma_j \mathbf{d}_j = -e\Sigma_j \mathbf{r}_j$ being the E1 operator with j^{th} electron at position \mathbf{r}_j .

Furthermore, the oscillator strengths f_{kv} for the corresponding transitions can be determined by [17,18]

$$f_{kv}^{E1} = \frac{1}{3\alpha} \left(\frac{\alpha \sigma}{R_{\infty}} \right) \times \frac{S^{E1}}{g_k} = \frac{303.756}{g_k \lambda} \times S^{E1}.$$
 (2)

The radiative lifetime (τ) of electronic state v can be estimated by reciprocating the total transition probability evaluated by the addition of the individual transition probabilities of the transitions from the upper electronic state (v) to each possible lower electronic state (k) [20], viz.,

$$\tau_v = \frac{1}{\Sigma_k A_{vk}^{E1}}.$$
(3)

Substituting A_{vk}^{E1} values from Equation (1), τ can be given in *s*.

3. Method of Evaluation

The accurate determination of atomic wave functions is limited by the presence of two-body electromagnetic interactions between electrons. Therefore, in this work we include the electron correlations due to the core-polarization effects through random-phase approximation (RPA); pair-correlation effects through the Brückner orbitals (BOs) and their couplings through the structural radiations (SRs) have been implemented. Moreover, the corrections in the results due to normalization of the wave functions (Norms) have been implemented explicitly. We refer to ref. [21] for detailed understanding of this method, however, a glimpse of the same is provided below.

Starting with the "no-pair" Hamiltonian $H = H_0 + V_I$, with H_0 and V_I being Dirac– Fock (DF), Hamiltonian and residual interaction [21–23], respectively, the mean-field wave function ($|\Phi_0\rangle$) of the $[4p^6]$ configuration of the considered ions is first evaluated. The corrections of the DF wave functions due to the electron correlation effects are estimated using the perturbative analysis of residual interaction by expressing the exact wave function of the state ($|\Psi_v\rangle$) in RMBPT as

$$|\Psi_v\rangle = |\Phi_v\rangle + |\Phi_v^{(1)}\rangle + |\Phi_v^{(2)}\rangle + \cdots$$
(4)

and the energy (E_v) as

$$E_v = E_v^{(0)} + E_v^{(1)} + E_v^{(2)} + \cdots,$$
(5)

where superscripts k = 1, 2, etc., represent the order of perturbation and $E_v^{(0)} = \sum_k^N \epsilon_k$ is the zeroth-order energy. Further employing these wave functions, the E1 matrix element between the states $|\Psi_v\rangle$ and $|\Psi_w\rangle$ is calculated as

$$D_{wv} = \frac{\langle \Psi_w | D | \Psi_v \rangle}{\sqrt{\langle \Psi_w | \Psi_w \rangle \langle \Psi_v | \Psi_v \rangle}}.$$
(6)

The above-stated matrix element incorporates the contributions from the perturbative corrections, including RPA, BO, SR and Norm. Consequently, the matrix element D_{wv} can be written as [21,22]

$$D_{wv} = D_{wv}^{DF} + D_{wv}^{RPA} + D_{wv}^{BO} + D_{wv}^{SR} + D_{wv}^{Norm},$$
(7)

where $D_{wv}^{DF} \equiv d_{wv} = \langle \phi_w | D | \phi_v \rangle$, with the DF single particle wave functions $|\phi_v\rangle$ and $|\phi_w\rangle$. Since core-polarization effects contribute significantly, they are included through RPA self-consistently to all orders [22,24]. The leading-order electron correlation contributions through BO and SR arise at the third-order perturbation level. The corresponding set of contributions have been included using the strategy followed by Johnson et al. in [22] for our respective calculations. Norm contributions have been estimated by following the approach of Blundell et al. [21].

Our procedure incorporates various physical effects due to the electron correlation effects that are completed through the third-order perturbation and core-polarization effects upon all orders.

4. Results and Discussion

We have provided detailed discussion of our calculated ionization energies, line strengths, transition probabilities and oscillator strengths of the considered ions in our work. Here, the reported values of line strengths, transition probabilities and oscillator strengths are calculated using the length gauge. We have also determined the lifetimes of $5P_{1/2,3/2}$ and $6S_{1/2}$ states of Tc VII, Ru VIII and Rh IX ions. During computation, it was observed that our calculated E1 matrix elements, using the RMBPT method for both length and velocity gauges, are in good agreement with the maximum number of transitions for all the considered ions, which further confirms the reliability of our calculated results.

Moreover, the relative differences in the results obtained using L- and V-gauge expressions are included as uncertainties.

In Table 1, we have tabulated ionization energies (IEs) of all the considered states of these ions, compared with energies derived from the available literature. Through Table 1, we saw a trend of decreasing IEs towards higher energy levels. It was observed that the IEs obtained for Tc VII ion using RMBPT vary less than 2% from the IEs obtained using the relativistic coupled-cluster (RCC) method in ref. [14]. It was also observed that the maximum and minimum IE variations are seen in $4D_{5/2}$ and $6S_{1/2}$ states with a variation of 1.17% and 0.39%, respectively. Moreover, the variation in IEs decreases towards the high-lying states. However, no explicit IE values have been found for Ru VIII and Rh IX ions. Additionally, we did not find any experimental energy values in the literature to compare our data with.

The obtained results for line strengths (S_{vk}), transition probabilities (A_{vk}) and oscillator strengths (f_{kv}) for Tc VII ion have been listed in Table 2. We have presented line strengths in length gauge, however, the uncertainties in our results have been approximated by implementing the differences in line strengths, obtained by using both L- and V-gauge expressions. The uncertainties (quoted in parentheses) for these spectroscopic properties have been evaluated using the uncertainties in E1 matrix elements. According to Table 2, the maximum transition probability is in the transition occurring between ground and first excited state, which is consistent with expectations for any ionic system. It is also analyzed that $4D_{3/2}$ – $6P_{1/2}$ transition shows maximum variation (~30%) in oscillator strength, which may be due to large electron correlation effects exhibited in these states, thereby questioning the reliability of this particular transition.

In Table 3, we have tabulated the radiative properties for Ru VIII ion. As expected, the maximum transition probability is seen for the $4D_{3/2}$ – $5P_{1/2}$ transition. Moreover, it is observed that the uncertainties in A_{vk} and f_{kv} values are considerably low except for $4D_{3/2,5/2}$ – $6P_{1/2,3/2}$ transitions. Unusually large uncertainties were observed for these three transitions, thereby making them unreliable for further analysis. The investigation of data obtained for these particular transitions demonstrated that the large errors are the consequence of the cancellation of contributions from DF with RPA, leading to very small resultant electric dipole matrix elements in V-gauge. Thus, the final uncertainty reflected in A_{vk} and f_{kv} values of these transitions is considerably large.

Table 4 presents the radiative results for Rh IX ion. Rh IX ion exhibits the same behaviour as Tc VII and Ru VIII ions with maximum A_{vk} for $4D_{3/2}$ – $5P_{1/2}$ transition. All transitions except $4D_{3/2}$ – $6P_{3/2}$ transition show small uncertainties in the radiative properties. Also, the transition wavelength for $6S_{1/2}$ – $6P_{1/2}$ transition is observed to be the largest which is particularly the same behaviour also shown previously by Tc VII and Ru VIII ions. Further, an unreasonably high uncertainty of 23% is observed in oscillator strength of $4D_{3/2}$ – $6P_{3/2}$ transition which is the consequence of high electronic correlations among these states. Nonetheless, the estimated uncertainties in these transitions are still reasonable for prospective astrophysical studies.

Table 5 tabulates the comparison of our results for oscillator strengths with available theoretical literature, demonstrating <10% variation with respect to the RCC results published in ref. [14]. Around 20% variation was seen against the results obtained by implementing core polarization effects on DF values by Migdalek in ref. [15]. Our results incorporate higher-order corrections as well as the contributions of core-polarization, which are neglected in the study discussed in ref. [15]. This further confirms the improved accuracy of our results. However, our results disagree with the results obtained by Zilitis [16]. This is due to the fact that the results given in ref. [16] are based only on the DF level, neglecting other strong contributions. During this study, we have seen that core-polarization as well as other effects contribute strongly to these transition properties and hence must be included. This is why the disparities between the results from both studies appear.

We have tabulated radiative lifetimes (τ) of 5 $P_{1/2,3/2}$ and 6 $S_{1/2}$ states of Tc VII, Ru VIII and Rh IX ions along with their comparison in Table 6. Less than 9% variation appears

in τ values of the considered states of Tc VII ions compared to the results obtained by Das et al. [14], which is within the error limit of 10%. Unfortunately, we do not find any literature to compare the obtained lifetimes of these states in ruthenium (Ru VIII) and rhodium (Rh IX) ions. For all three ions, a trend of decreasing lifetime is seen from $6S_{1/2}$, $5P_{1/2}$ to $5P_{3/2}$ states, reflecting the easy decay of electrons from $5P_{3/2}$ state.

The unavailability of data for the states above $6S_{1/2}$ in Tc VII and $5P_{3/2}$ in Ru VIII and Rh IX ions calls for further theoretical and experimental studies in order to validate our results thoroughly. Previously, only a small number of data were available and their uncertainties were not quoted. Our reported values will be useful for the analysis of various astrophysical processes involving Tc VII, Ru VIII and Rh IX ions. We believe that our estimated values for various radiative properties are more reliable, as our study involves all the necessary corrections from third-order perturbation theory.

ground state ionization limit is taken from NIST AD [25]. Ionization Energies (in cm^{-1})

Table 1. Ionization energies (cm⁻¹) for few, low lying and excited states using RMBPT method for Tc VII, Ru VIII and Rh IX, compared with RCC ionization energies provided by Das et al. [14]. The

Clata		101112411		, ,	
State	Tc VII	Ref. [14]	$\delta(\%)$	Ru VIII	Rh IX
$4D_{5/2}$	706,674.22	714,936.68	1.17	882,703.62	1,083,600.08
$5S_{1/2}$	544,578.06	550,080.50	1.01	666,540.74	808,192.47
$5P_{1/2}$	473,976.25	477,209.30	0.68	586,449.02	718,629.58
$5P_{3/2}$	467,743.91	470,667.03	0.62	578,440.90	708,584.25
$6S_{1/2}$	311,642.84	310,434.72	0.39	386,067.12	477,082.16
$6P_{1/2}$	280,145.08			349,587.13	435,563.73
6P _{3/2}	277,356.01			345,940.98	430,919.84

Table 2. The L-gauge line strengths ($S_{L_{nk}}$) (in a.u.), wavelengths (λ) (in Å), transition probabilities $(A_{L_{vk}})$ in (s^{-1}) and absorption oscillator strengths $(f_{L_{kv}})$ for the Tc VII ion through E1 decay channel. Values in square brackets represent the order of 10. Uncertainties are given in parentheses.

Upper State (v)	Lower State (k)	λ (in Å)	$S_{L_{vk}}$ (in a.u.)	$A_{L_{vk}}$ (in s^{-1})	$f_{L_{kv}}$
$5P_{1/2}$	$4D_{3/2}$	423.69	7.21[-1]	9.61(33)[9]	1.29(3)[-1]
$5P_{1/2}$	$5S_{1/2}$	1416.39	2.55[0]	9.08(29)[8]	2.73(4)[-1]
$5P_{3/2}$	$4D_{3/2}$	412.79	1.36[-1]	9.80(33)[8]	2.50(5)[-2]
$5P_{3/2}$	$4D_{5/2}$	418.53	1.28[0]	8.81(30)[9]	1.54(3)[-1]
$5P_{3/2}$	$5S_{1/2}$	1301.50	5.12[0]	1.18(3)[9]	5.97(11)[-1]
$6S_{1/2}$	$5P_{1/2}$	616.02	7.48[-1]	3.24(11)[9]	1.84(3)[-1]
$6S_{1/2}$	$5P_{3/2}$	640.61	$1.71[0]^{-1}$	6.58(21)[9]	2.03(3)[-1]
$6P_{1/2}$	$4D_{3/2}$	232.64	2.09[-2]	1.68(51)[9]	7(2)[-3]
$6P_{1/2}$	$5S_{1/2}$	378.17	7.92[-2]	1.48(6)[9]	3.18(6)[-2]
$6P_{1/2}$	$6S_{1/2}$	3174.83	8.97[0]	2.84(9)[8]	4.29(4)[-1]
$6P_{3/2}$	$4D_{3/2}$	231.14	5.51[-3]	2.26(37)[8]	1.81(29)[-3]
$6P_{3/2}$	$4D_{5/2}$	232.93	4.85[-2]	1.95(34)[9]	1.05(18)[-2]
$6P_{3/2}$	$5S_{1/2}$	374.22	1.16[-1]	1.12(5)[9]	4.71(18)[-2]
$6P_{3/2}$	$6S_{1/2}$	2916.57	1.79[1]	3.65(11)[8]	9.30(9)[-1]

Upper State (v)	Lower State (k)	λ (in Å)	$S_{L_{vk}}$ (in a.u.)	$A_{L_{vk}}$ (in s ⁻¹)	$f_{L_{kv}}$
$5P_{1/2}$	$4D_{3/2}$	332.72	5.64[-1]	1.55(5)[10]	1.29(1)[-1]
$5P_{1/2}$	$5S_{1/2}$	1248.57	2.18[0]	1.14(3)[9]	2.65(3)[-1]
$5P_{3/2}$	$4D_{3/2}$	324.09	1.06[-1]	1.58(5)[9]	2.48(2)[-2]
$5P_{3/2}$	$4D_{5/2}$	328.66	9.99[-1]	1.43(4)[10]	1.54(2)[-1]
$5P_{3/2}$	$5S_{1/2}$	1135.08	4.38[0]	1.52(5)[9]	5.87(6)[-1]
$6S_{1/2}$	$5P_{1/2}$	499.05	6.04[-1]	4.92(15)[9]	1.84(2)[-1]
$6S_{1/2}$	$5P_{3/2}$	519.82	1.39[0]	1.00(3)[10]	2.03(2)[-1]
$6P_{1/2}$	$4D_{3/2}$	186.08	7.19[-2]	1(2)[10]	3(6)[-2]
$6P_{1/2}$	$5S_{1/2}$	315.50	8.49[-2]	2.74(16)[9]	4.09(21)[-2]
$6P_{1/2}$	$6S_{1/2}$	2741.23	7.38[0]	3.63(14)[8]	4.09(10)[-1]
$6P_{3/2}$	$4D_{3/2}$	184.82	2.79[-3]	2(4)[8]	1(2)[-3]
$6P_{3/2}$	$4D_{5/2}$	186.30	4.58[-4]	4(30)[7]	1(11)[-4]
$6P_{3/2}$	$5S_{1/2}$	311.92	1.28[-1]	2.13(8)[9]	6.21(15)[-2]
6P _{3/2}	$6S_{1/2}$	2492.14	$1.49[1]^{2}$	4.68(16)[8]	9.05(15)[-1]

Table 3. The L-gauge line strengths $(S_{L_{vk}})$ (in a.u.), wavelengths (λ) (in Å), transition probabilities $(A_{L_{vk}})$ in (s^{-1}) and absorption oscillator strengths $(f_{L_{kv}})$ for the Ru VIII ion through E1 decay channel. Values in square brackets represent the order of 10. Uncertainties are given in parentheses.

Table 4. The L-gauge line strengths $(S_{L_{vk}})$ (in a.u.), wavelengths (λ) (in Å), transition probabilities $(A_{L_{vk}})$ in (s⁻¹) and absorption oscillator strengths $(f_{L_{kv}})$ for the Rh IX ion through E1 decay channel. Values in square brackets represent the order of 10. Uncertainties are given in parentheses.

Upper State (v)	Lower State (k)	λ (in Å)	$S_{L_{vk}}$ (in a.u.)	$A_{L_{vk}}$ (in s ⁻¹)	$f_{L_{kv}}$
$5P_{1/2}$	$4D_{3/2}$	270.00	4.53[-1]	2.33(7)[10]	1.27(1)[-1]
$5P_{1/2}$	$5S_{1/2}$	1116.53	1.90[0]	1.38(4)[9]	2.58(4)[-1]
$5P_{3/2}$	$4D_{3/2}$	262.87	8.20[-2]	2.29(7)[9]	2.37(3)[-2]
$5P_{3/2}$	$4D_{5/2}$	266.66	8.14[-1]	2.17(7)[10]	1.55(2)[-1]
$5P_{3/2}$	$5S_{1/2}$	1003.93	3.81[0]	1.91(6)[9]	5.77(7)[-1]
$6S_{1/2}$	$5P_{1/2}$	414.00	5.00[-1]	7.14(22)[9]	1.83(2)[-1]
$6S_{1/2}$	$5P_{3/2}$	431.96	1.16[0]	1.46(4)[10]	2.04(2)[-1]
$6P_{1/2}$	$4D_{3/2}$	153.04	5.69[-2]	1.61(41)[10]	2.82(72)[-2]
$6P_{1/2}$	$5S_{1/2}$	268.36	1.23[-1]	6.47(93)[9]	6.98(99)[-2]
$6P_{1/2}$	$6S_{1/2}$	2408.57	6.35[0]	4.60(31)[8]	4.00(25)[-1]
$6P_{3/2}$	$4D_{3/2}$	151.96	1.14[-2]	1.64(38)[9]	6(1)[-3]
$6P_{3/2}$	$4D_{5/2}$	153.21	9.01[-2]	1.27(26)[10]	2.98(60)[-2]
$6P_{3/2}$	$5S_{1/2}$	265.06	1.46[-1]	3.97(27)[9]	8.36(52)[-2]
6P _{3/2}	6S _{1/2}	2166.27	1.27[1]	6.34(33)[8]	8.92(40)[-1]

Table 5. Comparison of the oscillator strengths for Tc VII, Ru VIII and Rh IX ions from our calculations with available theoretical data. Uncertainties are given in parentheses.

Transition	Ion	$f_{L_{tra}}$			
		Present	[14]	B	[16]
$4D_{3/2} \rightarrow 5P_{1/2}$	Tc VII	0.129(3)	0.135	0.154	0.157
	Ru VIII	0.129(1)		0.153	
	Rh IX	0.127(1)		0.149	
$4D_{3/2} \rightarrow 5P_{3/2}$	Tc VII	0.0250(5)	0.026	0.030	0.0296
-//-	Ru VIII	0.0248(2)		0.0286	
	Rh IX	0.0237(3)		0.0276	
$4D_{5/2} \rightarrow 5P_{3/2}$	Tc VII	0.154(3)	0.161	0.183	
$5S_{1/2} \rightarrow 5P_{1/2}$	Tc VII	0.265(3)	0.290	0.277	0.367
-//-	Ru VIII	0.265(3)			0.357
	Rh IX	0.258(4)			0.348
$5S_{1/2} \rightarrow 5P_{3/2}$	Tc VII	0.597(11)	0.635	0.608	0.798
	Ru VIII	0.587(6)			0.787
	Rh IX	0.577(7)			0.775
$5P_{1/2} \rightarrow 6S_{1/2}$	Tc VII	0.184(3)	0.196	0.195	
$5P_{3/2} \rightarrow 6S_{1/2}$	Tc VII	0.203(3)	0.215	0.214	
$6S_{1/2} \rightarrow 6P_{1/2}$	Tc VII	0.429(4)		0.432	
$6S_{1/2} \rightarrow 6P_{3/2}$	Tc VII	0.930(9)		0.935	

State	Tc VII	Ru VIII	Rh IX
5P _{1/2}	95(3)	60(2)	41(1)
	86.90 [14], 76.80 [16]	49.60 [16]	34.00 [16]
$5P_{3/2}$	91.16(43)	57.47(22)	39(1)
	83.00 [14] <i>,</i> 75.30 [16]	49.00 [16]	33.9 [16]
$6S_{1/2}$	102(5)	67(2)	46(1)

Table 6. The estimated lifetimes τ (in ps) for $5P_{1/2,3/2}$ and $6S_{1/2}$ states of Tc VII, Ru VIII and Rh IX ions and their values from available data in the literature. Uncertainties are given in parentheses.

5. Conclusions

In this work, we have reported a number of radiative properties of Tc VII, Ru VIII and Rh IX ions by employing relativistic many-body perturbation theory involving all the necessary corrections through third-order perturbation theory. This study consists of precise estimations for line strengths, transition probabilities and absorption oscillator strengths for a total of 42 transitions of these three ions, as well as the radiative lifetimes of $5P_{1/2,3/2}$ and $6S_{1/2}$ states of these ions. A total of 14 transitions were considered for each of these ions occurring between all allowed $nD_{3/2,5/2}$, $n'S_{1/2}$ and $n'P_{1/2,3/2}$ states with n = 4 and n' = 5, 6. We have also compared our results with the previously reported values for a few selected transitions and observed a reasonably good agreement among them, with the exception of the study carried out by Zilitis [16]. Due to the scarcity of theoretical data, we call for further theoretical and experimental investigations to confirm these results. Our results with the quoted uncertainties can provide the desired benchmark for further studies in many astrophysical processes and their future applications.

Author Contributions: J. conceived the idea of calculating radiative properties of these ions on the basis of their astrophysical applications. J. calculated the spectroscopic data and drafted the manuscript. M.K. verified the results and contributed in the editing of the manuscript. B.A. provided critical feedback and helped shape the research, analysis and manuscript. She also aided in interpretation and discussion of the results and commented on the manuscript. M.K. and B.A. helped with writing the final draft of this manuscript. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The data underlying this article are available in the article.

Acknowledgments: Research at Perimeter Institute is supported in part by the Government of Canada through the Department of Innovation, Science and Economic Development and by the Province of Ontario through the Ministry of Colleges and Universities. The employed relativistic many-body method was developed in the group of M. S. Safronova of the University of Delaware, USA.

Conflicts of Interest: The authors declare no conflict of interest.

References

- Palme, H.; Lodders, K.; Jones, A. 2.2—Solar System Abundances of the Elements. In *Treatise on Geochemistry*, 2nd ed.; Holland, H.D., Turekian, K.K., Eds.; Elsevier: Oxford, UK, 2014; pp. 15–36. [CrossRef]
- 2. Merrill, P.W. Technetium in the stars. Amer. Assoc. Advancement Sci. 1952, 115, 484.
- 3. Shetye, S.; Van Eck, S.; Goriely, S.; Siess, L.; Jorissen, A.; Escorza, A.; Van Winckel, H. Discovery of technetium-and niobium-rich S stars: The case for bitrinsic stars. *Astron. Astrophys.* **2020**, *635*, L6. [CrossRef]
- 4. Martin, I.; Lavín, C.; Barrientos, C. Fine-structure oscillator strengths for excited-state transitions in Cu-like ions. *Int. J. Quantum Chem.* **1992**, *44*, 465–474. [CrossRef]
- Ruffoni, M.; Den Hartog, E.; Lawler, J.; Brewer, N.; Lind, K.; Nave, G.; Pickering, J. Fe I oscillator strengths for the Gaia-ESO survey. *Mon. Not. R. Astron. Soc.* 2014, 441, 3127–3136. [CrossRef]
- 6. Wittkowski, M. Fundamental stellar parameters Technology roadmap for future interferometric facilities, Proceedings of the European Interferometry Initiative Workshop organized in the context of the 2005 Join European and National Astronomy Meeting "Distant Worlds", 6–8 July 2005, Liège University, Institute of Astrophysics, Edited by J. Surdej, D. Caro, and A. Detal. Bulletin de la Société Royale des Sciences de Liège 2005, 74, 165–181.

- Rauch, T.; Gamrath, S.; Quinet, P.; Löbling, L.; Hoyer, D.; Werner, K.; Demleitner, M. Stellar laboratories-VIII. New Zr iv–vii, Xe iv–v, and Xe vii oscillator strengths and the Al, Zr, and Xe abundances in the hot white dwarfs G191-B2B and RE 0503-289. *Astron. Astrophys.* 2017, 599, A142. [CrossRef]
- Glushkov, A.; Ambrosov, S.; Orlova, V.; Orlov, S.; Balan, A.; Serbov, N.; Dormostuchenko, G. Calculation and extrapolation of oscillator strengths in Rb-like, multiply charged ions. *Russ. Phys. J.* 1996, 39, 81–83. [CrossRef]
- Tayal, S. Breit-Pauli oscillator strengths and electron excitation collision strengths for Si VIII. Astron. Astrophys. 2012, 541, A61. [CrossRef]
- 10. Griem, H. *Spectral Line Broadening by Plasmas*; Pure and applied physics a series of monographs and textbooks; Academic Press: New York, NY, USA, 1974.
- 11. Zeippen, C. Radiative opacities for stellar envelopes. Phys. Scr. 1995, 1995, 43. [CrossRef]
- Orban, I.; Glans, P.; Altun, Z.; Lindroth, E.; Källberg, A.; Schuch, R. Determination of the recombination rate coefficients for Na-like Si IV forming Mg-like Si III. Astron. Astrophys. 2006, 459, 291–296. [CrossRef]
- 13. Alonso-Medina, A.; Colón, C. Stark broadening of Ca IV spectral lines of astrophysical interest. *Mon. Not. R. Astron. Soc.* 2014, 445, 1567–1574. [CrossRef]
- Das, A.; Bhowmik, A.; Dutta, N.N.; Majumder, S. Electron-correlation study of Y III-Tc VII ions using a relativistic coupled-cluster theory. J. Phys. At. Mol. Opt. Phys. 2017, 51, 025001. [CrossRef]
- 15. Migdalek, J. Core-polarization corrected Dirac-Fock computations of one-electron spectra in the rubidium isoelectronic sequence: Mo VI through Pb XLVI. *At. Data Nucl. Data Tables* **2021**, *142*, 101455. [CrossRef]
- Zilitis, V. Oscillator strengths and lifetimes of levels for ions of the rubidium isoelectronic sequence calculated by the Dirac-Fock method. Opt. Spectrosc. 2007, 103, 895–898. [CrossRef]
- 17. Kelleher, D.E.; Podobedova, L. Atomic transition probabilities of sodium and magnesium. A critical compilation. *J. Phys. Chem. Ref. Data* 2008, *37*, 267–706. [CrossRef]
- Aymar, M.; Coulombe, M. Theoretical transition probabilities and lifetimes in Kr I and Xe I spectra. *At. Data Nucl. Data Tables* 1978, 21, 537–566. [CrossRef]
- 19. Nahar, S. Atomic data from the Iron Project. VII. Radiative dipole transition probabilities for Fe II. *Astron. Astrophys.* **1995**, 293, 967–977.
- Qin, Z.; Zhao, J.; Liu, L. Energy levels, transition dipole moment, transition probabilities and radiative lifetimes for low-lying electronic states of PN. J. Quant. Spectrosc. Radiat. Transf. 2019, 227, 47–56. [CrossRef]
- 21. Blundell, S.; Guo, D.; Johnson, W.; Sapirstein, J. Formulas from first-, second-, and third-order perturbation theory for atoms with one valence electron. *At. Data Nucl. Data Tables* **1987**, *37*, 103–119. [CrossRef]
- 22. Johnson, W.; Liu, Z.; Sapirstein, J. Transition rates for lithium-like ions, sodium-like ions, and neutral alkali-metal atoms. *At. Data Nucl. Data Tables* **1996**, *64*, 279–300. [CrossRef]
- 23. Safronova, U.; Safronova, M.; Johnson, W. Excitation energies, hyperfine constants, E 1, E 2, and M 1 transition rates, and lifetimes of 6 s 2 n l states in Tl I and Pb II. *Phys. Rev. A* 2005, *71*, 052506. [CrossRef]
- 24. Johnson, W.R. Atomic Structure Theory; Springer: Berlin/Heidelberg, Germany, 2007.
- 25. Kramida, A.; Ralchenko, Y.; Reader, J.; NIST ASD Team. *NIST Atomic Spectra Database*; National Institute of Standards and Technology: Gaithersburg, MD, USA, 2008.