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Oscillator strength calculations in neutral technetium

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ABSTRACT

Ab initio multiconfiguration calculations are performed for the oscillator strengths of the $\lambda = 4238$, 4262 and 4297 Å Tc I resonance lines of astrophysical interest. Electron correlation is treated through multiconfiguration expansions built from elaborate correlation models, while relativistic effects are introduced in the perturbation Breit–Pauli approximation or in the multiconfiguration Dirac–Fock–Breit variational approach. The calculated *gf*-values are sensitively lower (≈30 per cent) than the values obtained with the pseudo-relativistic Hartree–Fock wavefunctions calculated from a parametric analysis of Tc I by Palmeri & Wyart. The inclusion of a core-polarization potential in the latter approach confirms the present ab initio results when different ionic cores are used for the different transition arrays. The strong lines of Tc I are revisited adopting this model, giving rise to a systematic reduction in the oscillator strength scale due to core polarization. The astrophysical implications are discussed.

Key words: astrochemistry – atomic data – line: identification – nuclear reactions, nucleosynthesis, abundances – stars: AGB and post-AGB.

1 INTRODUCTION

Technetium ($Z = 43$) has three long-lived isotopes, ^{97}Tc ($\tau_{1/2} = 2.6 \times 10^6$ yr), ^{98}Tc ($\tau_{1/2} = 1.5 \times 10^6$ yr) and ^{99}Tc ($\tau_{1/2} = 2.1 \times 10^5$ yr), as well as 20 short-lived isotopes and isomers. Isotope ^{99}Tc is a uranium fission product and an abundant by-product of the nuclear power plant industry, while ^{95}Tc is often used as a radioactive tracer. The radioactivity of the nuclei of all Tc isotopes is the principal cause for the scarcity of atomic spectroscopic experimental investigations. From the theoretical point of view, Tc I belongs to the 4d elements, all characterized by rather complex spectra due to strongly perturbed levels for which accurate wavefunctions are difficult to obtain (O'Malley & Beck 2003).

Despite the high astrophysical interest of this element, the literature on Tc I atomic data remained rather poor (Bozman, Meggers & Corliss 1967; Bozman, Corliss & Tech 1968; Wendlandt, Bauche & Luc 1977; Garstang 1981), until the recent interpretation of energy levels by Palmeri & Wyart (1999) using the Racah–Slater formalism implemented in Cowan's chain of programs (Cowan 1981). The wavefunctions obtained from the parametric analysis of Tc I levels have been used for a first systematic evaluation of transition probabilities (Palmeri & Wyart 1999). More recently, O'Malley & Beck (2003), motivated by the search of specific transitions that could be used for the detection of technetium using the 'atom trap trace analysis' technique, performed a theoretical study of Tc I lifetimes. In their work, however, O'Malley & Beck (2003) wrote that no reliable Tc I oscillator strengths exist, omitting the important contributions of Garstang (1981) and Palmeri & Wyart (1999).

For heavy neutral atoms such as Tc I, both intra-valence and core–valence correlation, together with relativistic corrections, should be taken into account for accurate atomic structure calculations (Biémont et al. 2000; O'Malley & Beck 2003). Their simultaneous treatment in a configuration-interaction (CI) scheme is difficult and requires extensive configuration mixing to be considered. Even large computers impose rather severe limitations on the number of interacting configurations that can be considered simultaneously in the relativistic scheme. In particular, the inclusion of core-polarization effects requires the consideration of a huge number of configurations with open shells, often prevented by computer limitations. In this respect, electron correlation included in the semi-empirical calculations of Palmeri & Wyart (1999) was 'limited'.

For the three strong resonance lines of Tc I of astrophysical interest ($\lambda = 4238$, 4262 and 4297 Å), connecting the ground state $4d^5 5s^2\ a^6S_{5/2}$ to the $4d^5 5s(a^7S)\ 5p\ z^6P^o_{3/2,5/2,7/2}$ levels, the reliability of a model potential approach implemented in an adaptation of the pseudo-relativistic Hartree–Fock code of Cowan (1981) for describing the core-polarization effects is tested through a detailed comparison with ab initio multiconfiguration calculations taking correlation effects into account through the explicit inclusion of tailored excitations in the configuration space, and including relativistic corrections in the perturbation Breit–Pauli approximation or in the multiconfiguration Dirac–Fock–Breit variational approach.

The astrophysical interest of Tc I is illustrated in Section 2. The computational strategy is described in Section 3 for the different

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correlation and relativistic models (MCHF+BP, MCDF, HFR+CP) focusing on the three resonance lines. The HFR+CP model is then applied for revisiting the oscillator strengths of the strong Tc I lines selected in the original work of Palmeri & Wyart (1999). The results are compared and discussed in Section 4.

2 ASTROPHYSICAL INTEREST OF TECHNETIUM LINES

After the first discovery of technetium lines in the spectra of the S-type star R Andromedae (Merrill 1952), there has been a lot of effort put in to a systematic search for Tc lines in many stellar spectra of various kinds, mostly M, S and C stars (see, for example, the summary of Little-Marenin & Little 1978). It was quickly realized that the lack of Tc I and Tc II lines in the spectra of stars might have some interesting implications. For instance, the lack of technetium lines in barium stars suggested that the observed s-process enhancements were produced more than half a million years ago (Little-Marenin & Little 1987), supporting the idea that the spectral peculiarities of these stars were probably related to their binary nature. More recently, the use of traditional and statistical line identification methods has indicated the presence of Tc I and perhaps Tc II in the spectra of the 'Przybylski twin' (Cowley et al. 2004).

As discussed in the survey by Jorissen (2003), the presence of Tc in a star may be considered as the most reliable signature of its asymptotic giant branch (AGB) nature. The Tc-poor/Tc-rich dichotomy hides a profound difference in the evolutionary status of these two kinds of S stars, and is at the origin of the extrinsic/intrinsic paradigm. An illustration of this dichotomy is given by Fig. 1, comparing the absorption spectra of two S stars around the Tc I line at λ4262.270 (Jorissen & Van Eck, private communication). The spectra of these two S stars are almost identical, but the Tc line is absent in the upper spectrum (S star Henize 143), while it is prominent in the lower spectrum (S star Henize 39) and reflects a genuine Tc overabundance due to s-process nucleosynthesis occurring inside this star. This technetium dichotomy in the 'Henize' sample of S stars is discussed in more detail by Van Eck & Jorissen (1999). From a quantitative point of view, synthetic spectra of S stars, combined with medium-resolution technetium spectra, have been used to derive technetium abundances that were compared with the predictions of AGB nucleosynthesis models by Van Eck et al. (2001).

In this context, reliable oscillator strengths for Tc I lines are undoubtedly needed. A first attempt at their evaluation was realized for a few lines in the pioneering work of Garstang (1981). As pointed out in the Introduction, a more systematic evaluation of transition probabilities for this element was performed by Palmeri & Wyart (1999) using wavefunctions obtained from a parametric analysis of the energy levels. The present work focuses on the use of more elaborate correlation models that can be compared with the radiative data obtained by O'Malley & Beck (2003) using a relativistic configuration-interaction approach (RCI) in a multiconfiguration Dirac–Fock (MCDF) radial basis.

3 COMPUTATIONAL STRATEGY

3.1 The multiconfiguration approaches

3.1.1 MCHF+BP calculations

The non-relativistic wavefunction $\Psi(\gamma LSM_L M_S \pi)$ for an atomic state labelled by the configuration γ and term LS is approximated

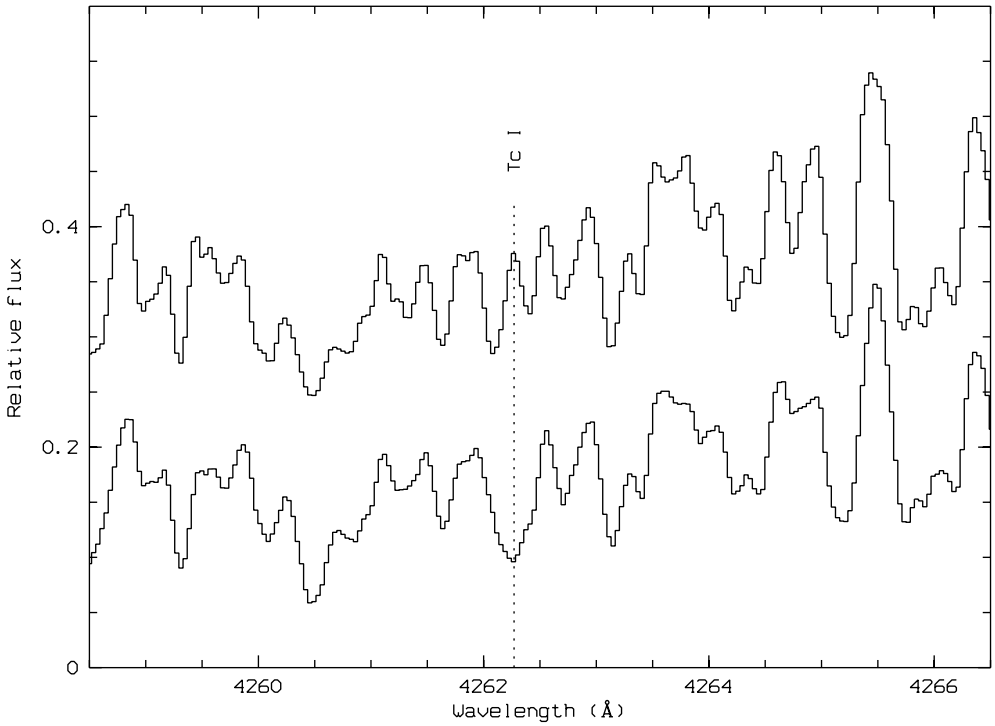

Figure 1. Comparison of high-resolution ($R = \lambda/\Delta\lambda = 60\,000$) absorption spectra of two S stars around the Tc I line at λ4262.270. Both spectra are normalized to the local pseudo-continuum but, for the sake of clarity, the upper spectrum is vertically shifted by 0.2 units with respect to the lower spectrum. The Tc line is absent in the upper spectrum (S star Henize 143), while it is prominent in the lower spectrum (S star Henize 39) and reflects a genuine Tc overabundance due to s-process nucleosynthesis occurring inside this star. The two spectra were obtained at the European Southern Observatory with the Coudé Echelle Spectrometer fed by the Coudé Auxiliary Telescope. They are part of a broader analysis of Tc in S stars (see Van Eck & Jorissen 1999).

by a linear combination of configuration state functions (CSFs),

$$\Psi(\gamma LSM_L M_S\pi) = \sum_{i=1} c_i \Phi(\gamma_i LSM_L M_S\pi). \quad (1)$$

Each $\Phi(\gamma_i LSM_L M_S\pi)$ is constructed from one-electron spin orbitals for the configuration γ_i and is of the same $(LSM_L M_S\pi)$ symmetry as the atomic state function. In the multiconfiguration Hartree–Fock (MCHF) method (Froese Fischer 1977, 2000), the one-electron numerical radial functions used to construct the CSFs and the expansion coefficients c_i are determined variationally so as to leave the non-relativistic energy stationary with respect to variations in the radial functions and the expansion coefficients. Once radial functions have been determined, a configuration-interaction calculation can be performed over the set of configuration states.

The one-electron orbital basis optimized using the non-relativistic MCHF variational approach can be used for building the configuration space in which the relativistic Breit–Pauli (BP) Hamiltonian is diagonalized. This defines the MCHF+BP method (Hibbert, Glass & Froese Fischer 1991; Froese Fischer, Brage & Jönsson 1997) in which the Hamiltonian includes the mass correction, the one- and two-body Darwin terms, the spin–spin contact term and the J-dependent spin–orbit, spin–other orbit and spin–spin interactions.

The intermediate coupling eigenvectors,

$$|\Psi(SLJM_J\pi)\rangle = \sum_i c_i |\Phi(\alpha_i S_i L_i JM_J\pi)\rangle, \quad (2)$$

resulting from the diagonalization of the Breit–Pauli Hamiltonian, another configuration-interaction problem, takes into account that J, M_J and π are the only 'good' quantum numbers, the operators $\boldsymbol{L}^2$ and $\boldsymbol{S}^2$ no longer commuting with the fine-structure operators.

For the present Tc I calculations, the MCHF configuration expansions (1) are built from the following configuration set:

$$[\mathrm{Kr}]4s^2 4p^6\{4d\}^3\{4d, 5s, 5p, 5d, 4f, 5g\}^2\{4d, 5s, \ldots, 6s, \ldots, 6g\}^2.$$

In this expansion, 4s and 4p are kept closed and there is a minimum of three electrons in the 4d subshell. In a way this is similar to a large single- and double-excitations (hereafter SD) multireference expansion using a multireference set taking the near-degeneracy of 4f and 5ℓ into account. For the MCHF optimization procedure, the selected roots of the configuration-interaction matrices are $4d^5 5s^2\ {}^6\mathrm{S}$ and $4d^5 5s5p\ {}^6\mathrm{P^o}$ for even and odd parity, respectively. All the one-electron radial functions of the spectroscopic and correlation orbitals are variational up to the $n = 5$ correlation model. In the last step, extending the orbital active set up to 6g, the $n \leqslant 3$ radial functions are kept frozen while the $n \geqslant 4$ orbitals are variational.

In the Breit–Pauli approximation, the effect of LS mixing is taken into account in the odd parity by mixing the $^6\mathrm{P^o}$ with the $^8\mathrm{P^o}$ and $^6\mathrm{D^o}$ terms. In the even-parity block, the mixing of $4d^5 5s^2\ {}^6\mathrm{S}$ and $4d^6 5s\ {}^6\mathrm{D}$ is found to be negligible, the mixing coefficient of the latter in the ground-state wavefunction being lower than 1×10^{-4}.

3.1.2 MCDF calculations

The multiconfiguration Dirac–Fock (MCDF) method is the fully relativistic counterpart (Grant 1996) to the non-relativistic MCHF scheme (Froese Fischer 1996). Here the Hamiltonian is given by

$$\sum_{i=1}^{N} \left[c\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + (\beta_i - 1)c^2 - \frac{Z}{r_i} \right] + \sum_{i<j}^{N} \frac{1}{r_{ij}}, \quad (3)$$

where c is the speed of light and $\boldsymbol{\alpha}$ and β are the Dirac matrices. The atomic wavefunction is given as an expansion over jj-coupled CSFs

$$|\Psi(JM_J\pi)\rangle = \sum_i c_i |\Phi(\alpha_i JM_J\pi)\rangle. \quad (4)$$

The CSFs in turn are constructed from Slater determinants built on the four-component Dirac orbitals

$$\phi(\boldsymbol{r}) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa m}(\hat{r}) \\ \mathrm{i}Q_{n\kappa}(r)\chi_{-\kappa m}(\hat{r}) \end{pmatrix}. \quad (5)$$

In the expression above, κ is the relativistic angular quantum number, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small component radial wavefunctions and $\chi_{\kappa m}(\hat{r})$ is the spinor spherical harmonic in the lsj coupling scheme

$$\chi_{\kappa m}(\hat{r}) = \sum_{m_l, m_s} \left\langle l\, \tfrac{1}{2} m_l m_s \mid jm \right\rangle Y_{lm_l}(\theta, \varphi)\xi_{m_s}(\sigma). \quad (6)$$

The relativistic package (GRASP92) is described by Parpia, Froese Fischer & Grant (1996). The MCDF expansions (4) are built including 'valence' correlation through single and double excitations from $\{4d^5 5s^2 + 4d^6 5s\}$ and $4d^5 5s5p$ for even and odd parity, respectively, extending the orbital active set up to $n = 5f$. The $n \leqslant 3$ core orbitals are taken from a Dirac–Fock calculation on $4d^5 5s^2\ {}^6\mathrm{S}_{5/2}$. The $n = 4$ and $n = 5$ orbitals are variational in both parities. For the even parity, we select an 'extended optimal level' (EOL) model (Dyall et al. 1989; Parpia et al. 1996) on the two lowest $J = 5/2$ ($4d^5 5s^2$ and $4d^6 5s$) atomic state functions. For the odd parity, we adopt the EOL model where three atomic state functions (the lowest root for $J = 3/2$ and the second roots of $J = 5/2$ and $J = 7/2$, respectively) are assigned their $(2J + 1)$ statistical weight.

3.2 The HFR+CP model potential approach

In the previous work of Palmeri & Wyart (1999), the pseudo-relativistic Hartree–Fock (HFR) option of the RCN code (Cowan 1981) was used to get the ab initio values of the Slater and spin–orbit integrals for two groups of mixed configurations ($4d^5 5s^2 + 4d^6 5s + 4d^7$) and ($4d^5 5s5p + 4d^6 5p + 4d^4 5s^2 5p$) that comprise the lower and upper levels of the strongest transitions of Tc I. The theoretical energies and eigenfunctions were determined by diagonalizing energy matrices of the mixed groups above, second-order effects of far configuration mixing being limited to the two-body operators described by the α and β parameters of d^N. The energy parameters were fitted with the largest possible number of experimental energies by means of the RCE code of Cowan's chain of programs (Cowan 1981). The weighted transition probabilities were then evaluated for a selection of strong emission lines, using the semi-empirical eigenvectors combined with the HFR radial transition integrals.

More extensive configuration mixing effects are considered in the present work. Outer correlation is indeed described by retaining configurations $4d^6 n$s, $4d^5 5sn$s, $4d^7$, $4d^6 5$d, $4d^5 5s5$d, $4d^4 5s^2 5$d, $4d^5 5p^2$ ($n = 5$–7) for the even parity and $4d^6 n$p, $4d^5 5sn$p, $4d^4 5s^2 5$p ($n = 5$–7) for the odd parity. Owing to computer memory limitations, however, the correlation level reached in a similar study of Cd-like ions (Biémont et al. 2000) could not be obtained. For example, Rydberg series such as $4d^5 5pn$p, $4d^5 5pn$s and $4d^5 5pn$d ($n > 5$), or other interaction effects within the complex like $4d^5 5d^2$, $4d^5 4f^2$, $4d^5 5f^2$ and $4d^5 5p5$d, are not explicitly taken into account.

Besides these intra-valence correlation excitations, core–valence correlation can be described through a core-polarization (CP) model potential implemented in Cowan's chain of programs (Biémont et al. 2000). This approach is referred to below as the HFR+CP model.

Hibbert (1982a,b, 1989) discussed a variety of different forms for this core-polarization potential. In the present paper, we adopt the following one-particle ($V_{\rm P1}$) and two-particle ($V_{\rm P2}$) operators, respectively, given by Migdalek & Baylis (1978)

$$V_{\rm P1} = -\tfrac{1}{2}\alpha_{\rm d}\sum_{i=1}^{n}\frac{r_i^2}{\left(r_i^2+r_{\rm c}^2\right)^3} \tag{7}$$

and

$$V_{\rm P2} = -\alpha_{\rm d}\sum_{i>j}^{n}\frac{\boldsymbol{r}_i\cdot\boldsymbol{r}_j}{\left[\left(r_i^2+r_{\rm c}^2\right)\left(r_j^2+r_{\rm c}^2\right)\right]^{3/2}}, \tag{8}$$

where n is the number of valence electrons, $\alpha_{\rm d}$ is the static dipole polarizability of the core and $r_{\rm c}$ is a suitable cut-off radius taken as the size of the ionic core. These core-polarization corrections are added in the potential term of the radial equations for the valence orbitals of the pseudo-relativistic Hartree–Fock (HFR) model of Cowan (1981).

A further correction was introduced by Hameed, Herzenberg & James (1968) and Hameed (1972), to allow for a more accurate treatment of the penetration of the core by the valence electrons. In the present formalism, this corresponds to the addition of the core-penetration term

$$\frac{1}{r_{\rm c}^3}\int_0^{r_{\rm c}} P_{nl}(r)r\,P_{n'l'}(r)\,{\rm d}r \tag{9}$$

to the integral

$$\int_0^{\infty} P_{nl}(r)\frac{r}{\left(r^2+r_{\rm c}^2\right)^{3/2}}P_{n'l'}(r)\,{\rm d}r, \tag{10}$$

for each one-electron radial integral appearing when integrating the two-body operator (8).

When including the core polarization and core penetration in the Hamiltonian, the dipole moment operator in the transition matrix element also has to be modified for consistency. The dipole radial integral

$$\int_0^{\infty} P_{nl}(r)r\,P_{n'l'}(r)\,{\rm d}r \tag{11}$$

has to be replaced by

$$\int_0^{\infty} P_{nl}(r)r\left[1-\frac{\alpha_{\rm d}}{\left(r^2+r_{\rm c}^2\right)^{3/2}}\right]P_{n'l'}(r)\,{\rm d}r - \frac{\alpha_{\rm d}}{r_{\rm c}^3}\int_0^{r_{\rm c}} P_{nl}(r)r\,P_{n'l'}(r)\,{\rm d}r. \tag{12}$$

Similar potentials have been used successfully for the description of not only nominal one- and two-electron atoms (Brage et al. 1993; Biémont et al. 2000) but also for more complex systems such as Ce II (Palmeri et al. 2000) [see e.g. Biémont & Quinet (2003) for a recent compilation of the lanthanide series].

The complexity of configurations with open 4d subshells and the experience acquired in a similar treatment in Lu I, another complex neutral system (Fedchak et al. 2000), suggest the use of two different core-polarization models: CP(1) and CP(2).

In the first one, CP(1), we consider seven valence electrons surrounding a Tc^{7+} core. The adopted core-polarization parameters are $1.42\,a_0^3$ for $\alpha_{\rm d}$ (Fraga, Karwowski & Saxena 1976) and $1.18\,a_0$ for $r_{\rm c}$, the ab initio HFR average value $\langle r\rangle$ for the outermost core orbital, $4p^6$.

In the second model, CP(2), different cores are used for the different types of configuration corresponding to different occupation numbers of the 4d subshell ($4d^7$, $4d^6$, $4d^5$ and $4d^4$). For the configuration $4d^7$, the core-polarization parameters are those used for CP(1). For the other configurations, we consider Tc^+, Tc^{2+} and Tc^{3+} cores, depending on the number of electrons in the 4d subshell, i.e. six, five or four electrons, respectively. The corresponding dipole polarizabilities of 16.19, 8.43 and $5.40\,a_0^3$ are taken from the tables of Fraga et al. (1976). The HFR average radii $\langle r\rangle$ for the 4d orbital calculated in each configuration are used as the cut-off radii in the potentials (7) and (8). As different core parameters are considered for the initial and the final configurations of each transition array, the arithmetic mean of $\alpha_{\rm d}$ values and the geometric mean of $r_{\rm c}$ values deduced respectively for the initial and the final configurations of a transition are used in equation (12) for the corrected E1-transition operator.

Using these core-polarization models combined with the Racah–Slater formalism implemented in Cowan's chain of programs (Cowan 1981), the eigenvectors resulting from the least-squares fitting procedure applied to get the best agreement between the calculated and the available experimental energy levels of Bozman et al. (1968) and Palmeri & Wyart (1999) are used for evaluating the transition probabilities.

4 DISCUSSION OF THE RESULTS

The oscillator strengths of the transitions $4d^55s^2\,a^6S_{5/2}$–$4d^55s(a^7S)\,5p\,z^6P^o_{3/2,5/2,7/2}$ are compared in Table 1 for the different models [MCHF+BP, MCDF, HFR+CP(1), HFR+CP(2)] and with the previous data available in the literature (Garstang 1981; Palmeri & Wyart 1999; O'Malley & Beck 2003).

For the MCHF+BP results, the length (l) and velocity (v) forms are reported, although only the length form, correct at the α^2 order, should be strictly kept in the Breit–Pauli formalism. A large discrepancy in the two forms would indicate either the neglect of important correlation effects, or large relativistic effects not taken into account using the non-relativistic form of the velocity transition operator. In the MCDF approximation, the Coulomb gauge (Grant 1974) is retained for comparison. Although the present MCHF+BP calculations definitely include more correlation than the MCDF calculations, by using not only a larger correlation orbital set but also by considering more excitations in the configuration space, the

Table 1. Comparison of oscillator strengths (*gf*-values).

Transition	λ (Å)	Previous studies				This work				
		G81[a]	PW99[b]	O'MB03[c]		MCDF	MCHF+BP		HFR+CP	
				l	v		l	v	CP(1)	CP(2)
$^6S_{5/2}$–$^6P^o_{7/2}$	4297.058	0.81	0.937	0.588	0.432	0.580	0.573	0.679	0.829	0.642
$^6S_{5/2}$–$^6P^o_{5/2}$	4262.270	0.59	0.647	0.426	0.306	0.420	0.397	0.461	0.574	0.447
$^6S_{5/2}$–$^6P^o_{3/2}$	4238.191	0.38	0.410	–	–	0.266	0.246	0.280	0.363	0.284

[a]Garstang (1981). [b]Palmeri & Wyart (1999). [c]O'Malley & Beck (2003).

Table 2. Oscillator strengths for selected strong lines of Tc I.

λ^a (Å)	Lower level[a]		Upper level[a]		Intensity[a]	$\log(gf)^b$
6625.573	16025	11/2	31114	9/2	500	−1.42
6130.805	15298	7/2	31605	7/2	1000	−1.20
6085.229	0	5/2	16428	5/2	800	−2.60
5924.468	0	5/2	16874	7/2	1000	−2.22
5642.132	15624	5/2	33343	3/2	1500	−0.83
5620.450	15298	7/2	33085	5/2	2000	−0.61
5589.019	14733	9/2	32620	7/2	3000	−0.36
5275.512	11578	3/2	30538	5/2	1000	−1.26
5161.810	13252	5/2	32620	7/2	2000	−0.68
5096.280	10516	7/2	30133	9/2	5000	−0.45
4891.918	11578	3/2	32014	5/2	8000	−0.41
4866.733	11063	5/2	31605	7/2	10000	−0.25
4853.588	10516	7/2	31114	9/2	20000	0.00
4740.608	10516	7/2	31605	7/2	10000	−0.40
4637.500	11063	5/2	32620	7/2	3000	−0.56
4522.841	10516	7/2	32620	7/2	10000	−0.23
4487.061	11063	5/2	33343	3/2	3000	−0.67
4297.058	0	5/2	23265	7/2	10000	−0.19
4262.270	0	5/2	23455	5/2	10000	−0.35
4238.191	0	5/2	23588	3/2	5000	−0.55
4176.276	4002	3/2	27940	5/2	1000	−0.80
4172.532	3700	5/2	27660	7/2	5000	−0.83
4170.274	4178	1/2	28151	3/2	4000	−0.93
4165.609	10516	7/2	34515	5/2	10000	−0.11
4145.080	4178	1/2	28296	1/2	3000	−1.38
4144.950	3250	7/2	27369	9/2	6000	−1.04
4124.217	3700	5/2	27940	5/2	8000	−0.89
4115.077	4002	3/2	28296	1/2	10000	−0.70
4095.668	3250	7/2	27660	7/2	15000	−0.34
4088.707	3700	5/2	28151	3/2	10000	−0.44
4049.108	3250	7/2	27940	5/2	10000	−0.34
4031.626	2572	9/2	27369	9/2	20000	0.07
3984.967	2572	9/2	27660	7/2	10000	−0.40
3779.373	4178	1/2	30630	3/2	2000	−0.74
3771.031	4178	1/2	30689	1/2	3000	−0.69
3768.774	4002	3/2	30528	5/2	5000	−0.38
3746.845	3700	5/2	30382	7/2	5000	−0.15
3718.861	3250	7/2	30133	9/2	10000	−0.02
3684.740	3250	7/2	30382	7/2	5000	−0.70
3636.070	2572	9/2	30067	11/2	10000	0.22
3635.146	4002	3/2	31503	3/2	3000	−0.63
3608.271	3700	5/2	31406	5/2	2000	−0.47
3550.645	3250	7/2	31406	5/2	4000	−0.54
3549.725	3250	7/2	31414	7/2	6000	−0.36
3466.278	2572	9/2	31414	7/2	5000	0.03
3183.108	0	5/2	31406	5/2	2000	−0.71
3182.367	0	5/2	31414	7/2	2000	−0.82
3173.295	0	5/2	31503	3/2	3000	−0.67
3131.233	0	5/2	31927	5/2	1500	−1.31
2615.873	0	5/2	38216	5/2	1000	0.25
2614.233	0	5/2	38240	7/2	1500	0.43
2608.855	0	5/2	38319	3/2	500	0.09

[a]Bozman et al. (1967, 1968).
[b]HFR+CP: calculation CP(2) (see the text).

agreement between the MCHF+BP (length formalism) and the MCDF *gf*-values is satisfactory. Moreover, the present length MCHF+BP *gf*-values agree with the length values (Babushkin gauge) reported by O'Malley & Beck (2003) within 7 per cent for the two $^6S_{5/2}$–$^6P^o_{7/2,5/2}$ lines (the third component of the multiplet was not considered by these authors, focusing on the $J = 5/2$–$11/2$ odd-parity levels).

While the theoretical HFR+CP oscillator strength values almost reproduce the theoretical results of Garstang (1981) when using the CP(1) model, the use of different cores in the CP(2) model substantially reduces the oscillator strengths, in agreement with the present ab initio results. Considering the 4d subshell in the ionic core of the HFR+CP(2) model seems to mimic successfully the interactions with configurations with excited 4d electrons like, for instance, $4d^35d^25s5p$ included in the MCDF and MCHF+BP models, but not in the CI expansion used in both CP(1) and CP(2) models. One can conclude that the *gf*-values of Palmeri & Wyart (1999) and Garstang (1981) are definitely too high and that the inclusion of a core-polarization potential in the HFR approach confirms the present ab initio results if different ionic cores are used for the different transition arrays. The latter observation is consistent with the effects found in Lu I (Fedchak et al. 2000), for which a similar core-polarization model, using different cores, with different polarizabilities and cut-off radii, had to be selected to get a good agreement between experimental and theoretical radiative lifetimes and branching fractions.

The strong lines of Tc I selected in the parametric study of Palmeri & Wyart (1999) are revisited in Table 2, according to the HFR+CP(2) model. These results are compared with those of Garstang (1981), Palmeri & Wyart (1999) and O'Malley & Beck (2003) in Figs 2, 3 and 4, respectively. The systematic deviation from the 'equality lines' appearing in Figs 2 and 3 illustrates the systematic reduction in the *gf*-values found when including the polarization effects. The scattering of the points on both sides of the equality line in Fig. 4, for which the above observed systematic deviation disappears, suggests a more satisfactory global distribution and agreement between the two sets of results, i.e. the present HFR+CP(2) and RCI data of O'Malley & Beck (2003).

From the atomic physics point of view, the present work contributes to a better understanding of the spectroscopy of the 4d elements. The systematic reduction found in the oscillator strength values using the HFR core-polarization model, relative to the previously published values (Palmeri & Wyart 1999), is large. The MCDF

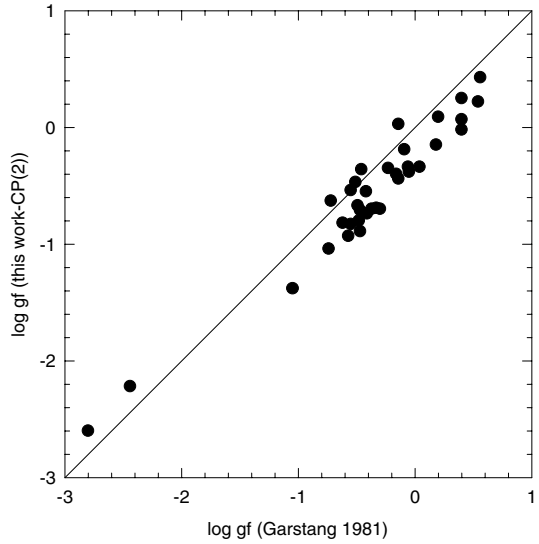

Figure 2. Comparison between the logarithm of the weighted oscillator strengths $\log(gf)$ reported in Table 2 of this work using CP(2) and those deduced from Garstang (1981).

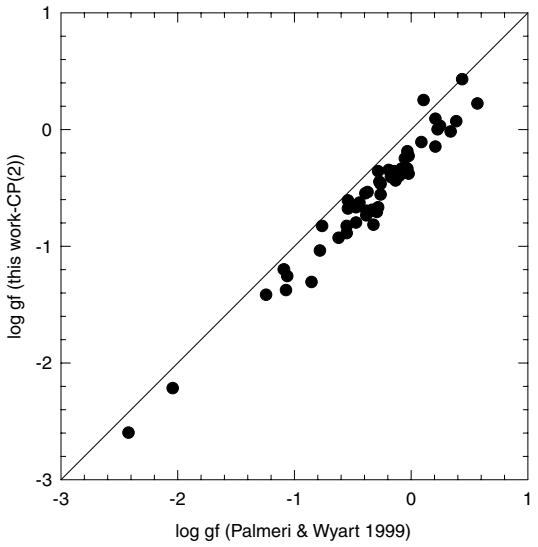

Figure 3. Same as Fig. 2, but with the results deduced from Palmeri & Wyart (1999).

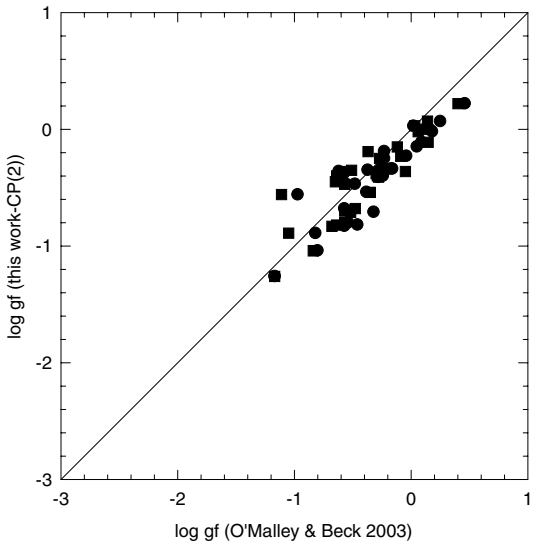

Figure 4. Same as Fig. 2, but with the results deduced from O'Malley & Beck (2003) (length, circles; velocity, squares).

and MCHF+BP calculations confirm the ≈30 per cent decrease found in the *gf*-values of the allowed $4d^5 5s^2\ a^6S_{5/2}$–$4d^5 5s\ (a^7S)\ 5p\ z^6P^o_{3/2,5/2,7/2}$ transitions. Experimental lifetimes and/or branching ratios can be used as interesting guidelines for the development of model potential methods, as illustrated by the recent work in Ce II (Palmeri et al. 2000; Zhang et al. 2001). The present work shows that robust ab initio calculations have their own place for such developments in cases for which experimental data are not available.

As far as astrophysical applications of the three $5s^2\ a^6S_{5/2}$–$5s5p\ z^6P^o_J$ lines are concerned, we recommend the use of the MCHF+BP *gf*-values (length formalism) reported in Table 1. A change in log(*gf*) has a direct impact on the stellar abundance of technetium. For the 4262 Å line, the reduction in the oscillator strength from the $gf = 0.647$ value reported by Palmeri & Wyart (1999) to the HFR+CP(2) $gf = 0.447$ value calculated in the present work corresponds to a decrease of 0.16 dex in the log(*gf*) scale. In the linear part of the curve of growth used to derive stellar abundances, this would then translate into a 0.16 dex increase in the technetium abundance. This is indeed the case for the S stars studied by Van Eck et al. (2001). This abundance shift is small with respect to the range of S-star technetium abundances expected from on-going nucleosynthesis (fig. 2 of Van Eck et al. 2001). It does not therefore alter the conclusions of that study comparing the observed abundances with predictions of AGB nucleosynthesis (Jorissen & Van Eck, private communication). The present work nevertheless provides accurate atomic data that should set future Tc abundance determinations on firmer grounds, and as such will be useful to the astrophysics community.

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