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Oscillator strengths for neutral selenium and tellurium

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Abstract. Oscillator strengths for excitations of neutral selenium and tellurium from the ground state are calculated using a semiempirical analytic independent-particle-model. The results are compared to experimental and theoretical data.

Key words: atomic data

1. Introduction

Oscillator strengths are needed as input data for calculations of chemical abundances in stellar objects. Although neutral selenium and tellurium (Se I and Te I) have not been observed in solar and star spectra, both elements are known to be present in meteorites, which may be inferred from the abundance tables of Anders and Grevesse (1989). These spectral observations may change in the light of data being collected by the Hubble Space Telescope high-resolution spectrometer (Leckrone et al. 1991). Oscillator strengths are also of interest in laboratory analytical spectroscopy. Selenium is known as a trace element in biology and agriculture. Both selenium and tellurium are used in semiconductor technology.

In this work we present the results of calculations of oscillator strengths for transitions from the ground states $4s^2 4p^4(^3P_2)$ of Se I and $5s^2 5p^4(^3P_2)$ of Te I. The many-body systems represented by Se I (34 electrons) and Te I (52 electrons) can be treated by an independent-particle-model in which each electron moves independently in an effective potential having the form

$$V(r) = -(2/r)\left\{(Z-1)\left[H(e^{r/d}-1)+1\right]^{-1}+1\right\} \qquad (1)$$

Here r is the electron-nucleus distance, and d, H are adjustable parameters. When this potential is substituted into the radial Schrodinger equation, the parameters d, H can be varied so that the energy eigenvalues agree with the experimental single-particle energy levels. The tables of Moore (1958) have an abundance of experimental energy levels from which singleparticle energies can be obtained by an averaging procedure described originally in the work of Ganas and Green (1971). The averaging procedure is performed only for triplet configurations such as ^3P, ^3D where the valence electron is coupled to a ^4S core. Quintet configurations such as ^5P, ^5D are excluded from these calculations. This is because the ground state is a triplet: $4s^2 4p^4(^3P_2)$, so that only those excited states that are triplets can be reached with a direct interaction. Excited states that are not triplets can only be reached by exchange interactions, and the present formalism does not make allowance for exchange interactions. We also exclude primed states such as s', p', which are coupled to a ^2D core, and s'', which is coupled to a ^2P core. A leastsquares search for the best values of the parameters d, H was performed and the following results were obtained: d = 0.9950, H = 5.0691 for Se I, and d = 0.7319, H = 3.1930 for Te I. The computed and experimental levels are in good agreement, as shown in Tables 1 and 2, the differences being less than 5%.

Table 1. Experimental and computed energy levels of Se I. Units are Rydbergs.

Level	Experimental	Computed
4p	0.7168	0.7184
5s	0.2521	0.2497
6s	0.1097	0.1090
7s	0.0617	0.0613
8s	0.0395	0.0393
9s	0.0275	0.0274
5p	0.1640	0.1626
6p	0.0824	0.0812
7p	0.0511	0.0490
8p	0.0320	0.0328
9p	0.0232	0.0235
4d	0.1216	0.1229
5d	0.0686	0.0686
6d	0.0438	0.0433
7d	0.0304	0.0297

2. Results and discussion

The general formula for computing oscillator strengths is standard. The computed values are given in Tables 3 and 4. Experimental and theoretical data are available for the resonance

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Table 2. Experimental and computed energy levels of Te I. Units are Rydbergs.

Level	Experimental	Computed
5p	0.6622	0.6682
6s	0.2371	0.2284
6p	0.1540	0.1571
7p	0.0791	0.0793
6d	0.0635	0.0672
7d	0.0406	0.0426
8d	0.0282	0.0294

Table 3. Present values of oscillator strengths for the transitions $4p^4$ ($^3P_2$) $\rightarrow$ $4p^3(^4S)$ ns ($^3S_1$) and $4p^4(^3P_2) \rightarrow 4p^3(^4S)$ nd (^3D) in Se I, and values from experiment and other calculations.

Final state	This calculation	Experiment	Other calculations
$5s(^3S_1)$	0.1167	0.1224 ± 0.0144[a]	0.1034[c], 0.1095[d], 0.112[e]
		0.074 ± 0.016[b]	0.136[e], 0.165[e], 0.062[f]
$6s(^3S_1)$	0.0188		
$7s(^3S_1)$	0.00678		
$8s(^3S_1)$	0.00326		
$9s(^3S_1)$	0.00183		
$4d(^3D_1)$	0.00309		
$4d(^3D_2)$	0.0464		
$4d(^3D_3)$	0.2598		
$5d(^3D_1)$	0.00125		
$5d(^3D_2)$	0.0188		
$5d(^3D_3)$	0.1053		
$6d(^3D_1)$	0.000599		
$6d(^3D_2)$	0.00898		
$6d(^3D_3)$	0.0503		
$7d(^3D_1)$	0.000328		
$7d(^3D_2)$	0.00492		
$7d(^3D_3)$	0.0276		

[a] Dynefors 1975, [b] Bengtsson et al. 1992, [c] Lawrence 1967, [d] Garpman et al. 1974, [e] Knox and Olechna 1967, [f] Gruzdev 1969

transitions 4p–5s (Se I) and 5p–6s (Te I), but no data, either experimental or theoretical, are available for any other transitions. For 4p–5s in Se I, the present calculated value 0.1167 lies inside the range of experimental values 0.1224 ± 0.0144 obtained by Dynefors (1975) and is only just outside the experimental range 0.074 ± 0.016 of Bengtsson et al. (1992). There are several theoretical results for 4p–5s. Lawrence (1967) obtained the value 0.1034 using an intermediate coupling theory, while Garpman et al. (1974) obtained the value 0.1095 using relativistic self-consistent-field radial wave functions in the Optimized Hartree-Fock-Slater scheme. A value 0.112 was obtained by Knox and Olechna (1967) using nonrelativistic Hartree- Fock theory. Our value is in excellent agreement with all of these theoretical values. Also included in Table 3 for comparison are two other values obtained by Knox and Olechna (1967), viz. 0.136, which is based on a dipole-velocity formula, and 0.165, which is based on a dipole-length formula with the matrix elements computed by Lawrence (1967). The value 0.112 of Knox and Olechna (1967) is a dipole-length value, as are all the present values. Another value, 0.062, was obtained by Gruzdev (1969) using a semi-empirical approximation in conjunction with an intermediate coupling scheme and the quantum defect method. His value is 60% of the value obtained by Lawrence (1967).

Table 4. Present values of oscillator strengths for the transitions $5p^4(^3P_2) \rightarrow 5p^3(^4S)$ ns ($^3S_1$) and $5p^4(^3P_2) \rightarrow 5p^3(^4S)$ nd (^3D) in Te I, and values from experiment and other calculations.

Final state	This calculation	Experiment	Other calculations
$6s(^3S_1)$	0.0987	0.098 ± 0.017[a]	0.1417[c], 0.070[d]
		0.1181 ± 0.0197[b]	
$7s(^3S_1)$	0.0181		
$8s(^3S_1)$	0.00675		
$9s(^3S_1)$	0.00330		
$10s(^3S_1)$	0.00224		
$5d(^3D_1)$	0.00295		
$5d(^3D_2)$	0.0442		
$5d(^3D_3)$	0.2475		
$6d(^3D_1)$	0.00127		
$6d(^3D_2)$	0.0190		
$6d(^3D_3)$	0.1065		
$7d(^3D_1)$	0.000624		
$7d(^3D_2)$	0.00936		
$7d(^3D_3)$	0.0524		
$8d(^3D_1)$	0.000347		
$8d(^3D_2)$	0.0052		
$8d(^3D_3)$	0.0291		

[a] Bengtason et al. 1992, [b] Dynefors 1975, [c] Garpman et al. 1974, [d] Gruzdev 1969

For the 5p–6s transition in Te I, the present value 0.0987 is in precise agreement with the experimental result 0.098 ± 0.017 of Bengtsson et al. (1992), and lies just inside the experimental range 0.1181 ± 0.0197 obtained by Dynefors (1975). It is also in reasonable agreement with the theoretical results 0.1417, obtained by Garpman et al. (1974), and 0.070, obtained by Gruzdev (1969).

It is interesting that the present results agree better with the experimental work of Dynefors (1975) than with the experimental work of Bengtsson et al. (1992) in the case of Se I and vice versa in the case of Te I. Dynefors (1975) uses a beamfoil technique, and states that the accuracy of his method is affected by appreciable cascading in heavy neutral elements. Since Te I is heavier than Se I, Dynefors' Te I result may be less accurate than his Se I result, which may explain why our calculations are in better agreement with his Se I result than with his Te I result. On the other hand, Bengtsson et al. (1992) use time-resolved laser spectroscopy, which is free from errors due to cascading. This suggests that the experimental value of Bengtsson et al. (1992) for Te I may be more accurate than Dynefors' (1975), thus explaining why our result for Te I is closer to Bengtsson et al.'s (1992) than to Dynefors' (1975). Another interesting observation is that when we compare the present results with those of Garpman et al. (1974), the agreement is much closer in the case of Se I than in the case of Te I. This may be attributed to relativis-

tic effects. Relativity is quite important in heavy atoms. Relativistic effects may be more appreciable in the heavier Te I atom than in the lighter Se I atom. Therefore relativistic wave functions may be more appropriate for Te I than the non-relativistic wave functions used in the present work.

3. Conclusion

The purpose of the present calculations has been to generate oscillator strengths for transitions of Se I and Te I from their ground states to various excited states. Reasonable to good agreements with experimental and theoretical data have been obtained for the resonance transition. Our results for the higher states are new since no experimental or theoretical information is available for them. We have attempted to gauge the accuracy of our results by comparing them to the ranges of experimental values obtained by Dynefors (1975) in the case of Se I, and Bengtsson et al. (1992) in the case of Te I, which we believe are the most accurate experimental results available. We find that our values are within 8% to 22% of the experimental values. Therefore we assign an accuracy anywhere from 8% to 22% to all of our oscillator strengths.

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