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Article

Calculated Transition Probabilities for Os VI Spectral Lines of Interest to Nuclear Fusion Research

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Abstract: In this work, we present a new set of transition probabilities for experimentally classified spectral lines in the Os VI spectrum. To do this, two independent computational approaches based on the pseudo-relativistic Hartree-Fock including core-polarization effects (HFR+CPOL) and fully relativistic Multiconfiguration Dirac-Hartree-Fock (MCDHF) methods were used, the detailed comparison of the results obtained with these two approaches allowing us to estimate the quality of the calculated radiative parameters. These atomic data, corresponding to 367 lines of five times ionized osmium between 438.720 and 1486.275 Å, are expected to be useful for the analysis of the spectra emitted by fusion plasmas in which osmium could appear as a result of transmutation by neutron bombardment of tungsten used as component of the reactor wall, such as the ITER divertor.

Keywords: atomic data; transition probabilities; fusion plasma diagnostics

1. Introduction

It is now well established that tungsten (W) will be widely used in nuclear fusion reactors as a plasma-facing material due to its high melting point, low sputtering yield, and resistance to neutron irradiation. In particular, tungsten will be a key material for the divertor of the International Thermonuclear Experimental Reactor (ITER), the component designed to manage heat and particle flux from the plasma [1–3]. During nuclear fusion operations, the divertor will endure some of the harshest conditions in the reactor. Thus, under neutron bombardment, tungsten will undergo nuclear transmutation, forming other elements, including osmium [4].

As a transmutation product of tungsten, osmium atoms will also be sprayed into the plasma, altering its composition. Monitoring osmium's spectroscopic signals will help in understanding the dynamics of plasma-wall interactions, which are crucial for predicting material erosion and plasma contamination. The high ionization potential of neutral osmium (8.4 eV) means its ionic species may survive in high-temperature plasmas, providing diagnostic data about plasma conditions. Spectral lines of Os ions will therefore be particularly useful for identifying impurity influx from plasma-facing components and the corresponding radiative decay rates will also be used to calculate essential plasma properties, such as electron temperature and density.

The main goal of the present work is to make a new contribution to this field by determining the transition probabilities for spectral lines of five times ionized osmium (Os VI) which is characterized by a moderately complex atomic structure with 71 electrons giving $5d^3\ 4F_{3/2}$ as the ground level. Spectroscopic studies have already been carried out previously for this ion. Indeed, nearly 30 years ago, Raassen *et al.* [5] classified 290 lines belonging to the $5d^3 - 5d^26p$ transition array in the 435 – 765 Å region and 87 lines belonging to the $5d^26s - 5d^26p$ transition array in the 940 – 1510 Å region from the analysis of spectrograms made by means of the 3.0 m and 10.6 m normal incidence spectrographs installed at that time in Antigonish (Canada) and Meudon (France). This resulted in the determination of all levels (19) in the $5d^3$ ground configuration, 14 levels (out of 16 possible) in the $5d^26s$ configuration and all levels (45) in the $5d^26p$ configuration. The analysis was guided by

predicted energy level values and transition probabilities calculated by means of a complete set of orthogonal operators. Calculated energy values, *LS*-compositions and *gA*-values, obtained from the fitted parameters using a rather limited configuration interaction model were also reported. More recently, Azarov [6] critically reviewed the data available on the $5d^3$, $5d^26s$ and $5d^26p$ configurations in the Lu I isoelectronic sequence, including Os VI, by means of calculations with orthogonal operators. This study allowed the determination of two new levels in the $5d^26s$ configuration of Os VI, namely $(^3P)^2P_{1/2}$ and $(^3P)^4P_{5/2}$.

If the electronic structure of the first three configurations of Os VI is now well known, the same cannot be said for the radiative parameters which have only been calculated by means of the pseudo-relativistic Hartree-Fock method (HFR) including the configuration interaction in a very limited way [5]. This motivated the present work, the objective of which is to provide a new set of reliable transition probabilities for experimentally observed spectral lines of Os VI. To do this, two independent methods were used, namely the pseudo-relativistic Hartree-Fock approach including core-polarization corrections (HFR+CPOL) and the fully relativistic Multiconfiguration Dirac-Hartree-Fock approach (MCDHF), the cross-comparison of the results obtained with these two methods allowing us to estimate the accuracy of the new calculated radiative data.

2. Computational Approaches

2.1. Pseudo-Relativistic Hartree-Fock Method with Core-Polarization Corrections

The first method used for computing the radiative rates in Os VI was the pseudo-relativistic Hartree-Fock (HFR) method, originally introduced by Cowan [7], modified for taking core-polarization effects into account, giving rise to the so-called HFR+CPOL method, as described e.g. in [8–10].

The physical model was chosen as consisting of three valence electrons surrounding an Os IX-type ionic core with 76 electrons. This led us to consider the valence-valence interactions by explicitly introducing the following configurations into the calculations : $5d^3 + 5d^26s + 5d6s^2 + 5d^26d + 5d6p^2 + 5d6d^2 + 5d5f^2 + 5d6f^2 + 5d6s6d + 5d6p5f + 5d6p6f + 5d5f6f + 6s^26d + 6s6p^2 + 6p^26d + 6s6d^2 + 6d^3 + 6s5f^2 + 6d5f^2 + 6s6f^2 + 6d6f^2$ for the even parity, and $5d^26p + 5d^25f + 5d^26f + 5d6s6p + 5d6s5f + 5d6s6f + 5d6p6d + 5d6d5f + 5d6d6f + 6s^26p + 6s^25f + 6s^26f + 6p^25f + 6p^26f + 6p^3 + 6p6d^2 + 6d^25f + 6d^26f + 6p5f^2 + 6p6f^2 + 5f^26f + 5f6f^2$ for the odd parity. This list of configurations is similar to the one considered for our recent HFR+CPOL calculations of radiative parameters in the isoelectronic ion Re V [11]. Core-valence interactions were then estimated using a core-polarization potential and a correction to the electric dipole operator, as described in [8–10], with a dipole polarizability $\alpha_d = 1.50 \text{ a}_0^3$ and a cut-off radius $r_c = 1.12 \text{ a}_0$, the former parameter being found by extrapolating the α_d -values published by Fraga *et al.* [12] for the first ions of the erbium isoelectronic sequence, i.e. Tm II, Yb III, Lu IV, and Hf V, while the latter parameter corresponds to the mean radius of the outermost orbital of the Os IX ionic core ($5p$), as obtained in the HFR calculations.

The HFR+CPOL calculations were then refined using a well-known least-squares fitting procedure of the computed energy levels to the experimental values available in the literature. More precisely, the experimental energy levels belonging to the $5d^3$, $5d^26s$ even configurations and the $5d^26p$ odd configuration published by Raassen *et al.* [5] were used to optimize the radial parameters corresponding to the average energies (E_{av}), the Slater integrals (F^k , G^k , R^k), the spin-orbit parameters (z_{nl}), and the effective interaction parameters a , b characterizing these three configurations. This led to average deviations between calculated and experimental energies of 46 cm^{-1} and 150 cm^{-1} for the odd and even parities, respectively. These deviations are slightly higher than those obtained in the fits made by Raassen *et al.* [5] (i.e. 11 and 107 cm^{-1}) and Azarov [6] (14 and 95 cm^{-1}) for the same configurations, but it should be noted that our calculations include a much larger number of interacting configurations, which often leads to slightly more complicated adjustment procedures, because of the more numerous mixtures in the eigenvector compositions. A detailed comparison between the HFR+CPOL levels and the available experimental values reported in [5,6] is given in

Table 1 in which the first two *LS*-components obtained in our calculations for each level are also listed. These eigenvector compositions are in excellent agreement with those published in [6].

Table 1. Comparison of the energy levels computed in the present work using the HFR+CPOL and MCDHF methods with the available experimental values for the 5d³, 5d²6s and 5d²6p configurations of Os VI. All values are given in cm⁻¹.

Conf.	Composition ¹	J	E _{EXP} ²	E _{HFR+CPOL}	DE _{HFR+CPOL}	E _{MCDHF}	DE _{MCDHF}
5d ³	81% ⁴ F + 10% ² D	1.5	0.0	0	0	0	0
	94% ⁴ F + 4% ² D	2.5	6397.4	6422	25	5912	-485
	84% ⁴ F + 13% ² G	3.5	11444.1	11450	6	11045	-399
	46% ⁴ P + 35% ² P	1.5	14430.2	14390	-40	15525	1095
	56% ⁴ F + 33% ² G	4.5	14678.3	14651	-27	14901	223
	68% ⁴ P + 32% ² P	0.5	16772.4	16806	34	17878	1106
	81% ² G + 15% ⁴ F	3.5	22919.6	22950	30	24181	1261
	56% ² H + 34% ⁴ F	4.5	24028.4	24054	26	25420	1392
	89% ⁴ P + 7% ² D	2.5	24828.5	24808	-20	25636	808
	42% ⁴ P + 34% ² D	1.5	27894.0	27944	50	28591	697
	67% ² P + 32% ⁴ P	0.5	28859.8	28876	16	29696	836
	100% ² H	5.5	32155.8	32159	3	34620	2464
	84% ² D + 6% ² D	2.5	34417.8	34433	15	35784	1366
	57% ² G + 32% ² H	4.5	37019.4	37011	-8	38308	1289
	85% ² F + 8% ² D	2.5	39600.8	39572	-29	43286	3685
	55% ² P + 17% ² D	1.5	40202.6	40186	-17	40607	404
	94% ² F + 5% ² G	3.5	40447.0	40455	8	43864	3417
	66% ² D + 33% ² D	1.5	59910.8	59972	61	63816	4005
	77% ² D + 12% ² F	2.5	61005.3	60968	-37	64058	3053
5d ² 6s	91% (³ F) ⁴ F + 8% (¹ D) ² D	1.5	97940.4	97929	-11	101568	3628
	78% (³ F) ⁴ F + 12% (³ F) ² F	2.5	100973.9	101053	79	104606	3632
	95% (³ F) ⁴ F + 5% (³ F) ² F	3.5	108538.4	108578	40	111778	3240
	53% (³ F) ² F + 21% (³ F) ⁴ F	2.5	114140.1	114133	-7	118083	3943
	90% (³ P) ⁴ P + 7% (¹ S) ² S	0.5	114363.2	114318	-45	119157	4794
	90% (³ F) ⁴ F + 10% (¹ G) ² G	4.5	115173.8	115184	10	118469	3295
	85% (³ P) ⁴ P + 12% (¹ D) ² D	1.5	118499.8	118478	-22	123014	4514
	51% (³ P) ⁴ P + 29% (³ F) ² F	2.5	119205.3	119259	54	123539	4334
	59% (¹ D) ² D + 21% (³ P) ² P	1.5	123318.6	123334	15	128060	4741
	61% (³ F) ² F + 36% (¹ G) ² G	3.5	123600.5	123520	-80	128038	4438
	90% (³ P) ² P + 5% (³ P) ⁴ P	0.5	129179.2	129417	238	134405	5226
	89% (¹ G) ² G + 10% (³ F) ⁴ F	4.5	130849.6	130957	107	136556	5706
	55% (¹ D) ² D + 39% (³ P) ⁴ P	2.5	131676.2	131632	-44	135923	4247
	63% (¹ G) ² G + 33% (³ F) ² F	3.5	132989.9	132897	-93	138231	5241
	77% (³ P) ² P + 19% (¹ D) ² D	1.5	138441.2	138555	114	143272	4831
	89% (¹ S) ² S + 5% (³ P) ² P	0.5	157388.9	157398	8	162297	4907
5d ² 6p	62% (³ F) ⁴ G + 19% (³ F) ² F	2.5	170473.6	170724	250	194287	23813
	48% (³ F) ⁴ F + 31% (³ F) ² D	1.5	175839.8	175579	-261	199974	24134
	72% (³ F) ⁴ G + 11% (³ F) ² F	3.5	182479.5	182524	44	205881	23401
	44% (³ F) ⁴ F + 20% (³ F) ² D	2.5	184033.0	184198	165	207833	23800
	50% (³ P) ⁴ D + 16% (³ P) ² S	0.5	186854.0	186757	-97	211679	24825
	36% (³ F) ⁴ G + 21% (³ F) ⁴ F	4.5	190882.5	190866	-17	214816	23933
	27% (³ P) ⁴ D + 21% (¹ D) ² P	1.5	190987.8	191141	153	215754	24766
	20% (³ F) ⁴ G + 13% (³ P) ⁴ D	2.5	191516.9	191381	-136	215489	23972

	39% (³ P) ² S + 33% (³ P) ⁴ P	0.5	192087.9	192468	380	216865	24777
	33% (³ F) ⁴ D + 31% (³ F) ⁴ F	3.5	192575.6	192473	-103	216520	23944
	35% (³ F) ⁴ F + 18% (³ F) ² D	1.5	194263.2	194306	43	217644	23381
	39% (³ P) ⁴ D + 21% (³ P) ⁴ S	1.5	195716.1	195276	-440	220433	24717
	24% (³ F) ² F + 20% (³ F) ⁴ D	2.5	196152.8	196100	-53	219905	23752
	33% (³ F) ² G + 17% (³ F) ⁴ G	3.5	197134.0	197161	27	220461	23327
	70% (³ F) ⁴ D + 13% (¹ D) ² P	0.5	198144.3	198214	70	222234	24090
	57% (³ F) ⁴ G + 18% (¹ G) ² G	4.5	202263.2	202190	-73	225816	23553
	46% (¹ G) ² G + 29% (³ F) ⁴ F	3.5	203069.9	203306	236	227580	24510
	18% (³ F) ² F + 18% (¹ D) ² F	2.5	204720.9	204779	58	228186	23465
	38% (³ P) ⁴ S + 20% (¹ D) ² P	1.5	205711.8	205702	-10	230358	24646
	20% (³ F) ² G + 18% (³ F) ² F	3.5	206193.4	206188	-5	230443	24250
	41% (³ F) ⁴ F + 34% (¹ G) ² H	4.5	206555.3	206346	-209	231212	24657
	29% (³ F) ² F + 28% (¹ D) ² F	2.5	207333.9	207247	-87	231344	24010
	55% (³ F) ⁴ D + 20% (³ F) ² D	1.5	207349.5	207473	123	230967	23617
	25% (³ F) ⁴ D + 17% (³ P) ⁴ D	3.5	209856.0	209916	60	233316	23460
	90% (³ F) ⁴ G + 10% (¹ G) ² H	5.5	210146.1	209870	-276	232910	22764
	60% (³ P) ⁴ P + 14% (³ P) ⁴ S	1.5	211634.7	211444	-191	236166	24531
	39% (³ P) ⁴ P + 28% (¹ D) ² P	0.5	212086.5	212047	-40	236322	24235
	25% (³ P) ⁴ D + 25% (³ F) ² D	2.5	214387.4	214508	121	238266	23879
	55% (³ F) ² G + 21% (³ F) ⁴ F	4.5	215369.6	215554	214	238802	23432
	42% (³ P) ⁴ P + 27% (¹ D) ² D	2.5	216397.1	216259	-138	240712	24315
	33% (³ P) ⁴ D + 16% (³ F) ⁴ D	3.5	216704.6	216785	80	240859	24154
	30% (¹ D) ² D + 27% (³ P) ² P	1.5	217361.9	217482	120	241850	24488
	53% (³ P) ² D + 14% (³ F) ² D	1.5	219500.4	219622	122	244276	24776
	36% (¹ D) ² P + 20% (³ P) ⁴ P	0.5	219979.0	219971	-8	244249	24270
	24% (¹ D) ² D + 23% (³ F) ² D	2.5	220744.9	220682	-63	245292	24547
	42% (¹ G) ² G + 33% (¹ G) ² H	4.5	221932.2	221965	33	246907	24975
	42% (³ P) ² P + 30% (¹ S) ² P	0.5	224004.9	224156	151	248952	24947
	41% (¹ D) ² F + 33% (³ P) ⁴ D	3.5	225818.9	225920	101	249663	23844
	89% (¹ G) ² H + 10% (³ F) ⁴ G	5.5	226320.5	226170	-150	251706	25386
	33% (¹ G) ² F + 18% (³ P) ² D	2.5	227935.6	228019	83	252758	24822
	47% (¹ G) ² F + 20% (¹ G) ² G	3.5	228256.2	228274	18	253798	25542
	48% (³ P) ² P + 16% (¹ D) ² D	1.5	231998.6	231890	-109	256680	24681
	55% (¹ G) ² F + 15% (³ F) ² D	2.5	233168.5	233242	74	258815	25647
	53% (¹ S) ² P + 26% (³ P) ² P	0.5	236614.5	236645	31	262090	25476
	87% (¹ S) ² P + 3% (³ P) ² D	1.5	252203.4	252163	-40	277153	24950

¹ Only the first two components, as computed in our HFR+CPOL model, are given. ² Experimental energy level values taken from [5,6].

2.2. Fully Relativistic Multiconfiguration Dirac-Hartree-Fock Method

The second computational approach used in the present work was the fully-relativistic Multiconfiguration Dirac-Hartree-Fock (MCDHF) method, as described in [13,14] and implemented in the latest version of the General Relativistic Atomic Structure Package, namely GRASP2018 [15].

We started our calculations by considering the 5d³, 5d²6s even- and the 5d²6p odd-parity configurations as the multireference (MR) with all the orbitals optimized on the 5d³ 4F_{3/2} ground state, in a first step, and then optimizing separately only the 5d and 6s orbitals on all the levels of the MR even configurations (5d³+5d²6s) and only the 5d and 6p orbitals on all the levels of the MR odd configuration 5d²6p. Thereafter, correlation orbitals were introduced and optimized layer by layer on all the levels of the MR in two steps in valence-valence (VV) expansions of the atomic state functions (ASFs) where all single and double (SD) excitations were allowed from the 5d, 6s and 6p spectroscopic

orbitals to the following orbital active sets (AS) where the set of $n_{\max}$ stands for the maximum value of the orbital principal quantum number for each azimuthal quantum number l : {7s,6p,6d,5f} and {6s,7p,6d,5f} for the even- and odd-parities, respectively, in a first step (VV1 model), and {8s,7p,7d,6f} and {7s,8p,7d,6f} for the even- and odd-parities, respectively, in a second step (VV2 model). Finally, core-valence (CV) and core-core (CC) correlations were considered in a relativistic configuration interaction (RCI) calculation using the orbitals optimized previously. Here, the ASF expansions were further extended by adding SD excitations from the 4f core orbital of the MR configurations to the AS of the last step of the orbital optimizations. This gave rise to 515 057 and 900 402 configuration state functions (CSFs) in the even- and odd-parities, respectively.

The final MCDHF energy levels are compared to the available experimental values in Table 1, where it can be seen that a fairly good agreement has been reached, the average deviation being equal to 8% for the whole set of energy levels belonging to the 5d³, 5d²6s and 5d²6p configurations, with a lower value for even-parity levels (4%) compared to the value obtained for odd-parity levels (10%).

3. Radiative Decay Rates

Transition probabilities (gA in 10¹⁰ s⁻¹) obtained in the present work with the HFR+CPOL and MCDHF methods are reported in Table 2. They are given for the lines experimentally identified by Raassen *et al.* [5] in the Os VI spectrum between 438.720 and 1486.275 Å. In this table, the transitions are classified by the numerical values of the lower and upper energy levels, with the spectroscopic designations of these levels given in Table 1. Transition probabilities published in [5] are also given for comparison in Table 2.

Table 2. Transition probabilities for experimentally observed lines in the Os VI emission spectrum.

l (Å) ¹	Lower level ²		Upper level ²		gA (10 ¹⁰ s ⁻¹)		
	E (cm ⁻¹)	J	E (cm ⁻¹)	J	Previous ³	HFR+CPOL ⁴	MCDHF ⁴
438.720	0.0	1.5	227935.6	2.5	0.006	0.006*	0.004
455.577	0.0	1.5	219500.4	1.5	0.068	0.061*	0.042
459.160	34417.8	2.5	252203.4	1.5	0.150	0.151	0.220
461.913	11444.1	3.5	227935.6	2.5	0.022	0.024*	0.022
466.531	6397.4	2.5	220744.9	2.5	0.092	0.087	0.053
469.251	6397.4	2.5	219500.4	1.5	0.017	0.025*	0.024
471.499	0.0	1.5	212086.5	0.5	0.025	0.023*	0.022
471.694	40202.6	1.5	252203.4	1.5	0.185	0.305	0.275
472.510	0.0	1.5	211634.7	1.5	0.069	0.070	0.044
473.616	14678.3	4.5	225818.9	3.5	0.061	0.071*	0.148
474.010	6397.4	2.5	217361.9	1.5	0.052	0.059*	0.041
475.490	6397.4	2.5	216704.6	3.5	0.007	0.011*	0.012**
475.625	22919.6	3.5	233168.5	2.5	0.104	0.095*	0.126
476.191	6397.4	2.5	216397.1	2.5	0.085	0.086*	0.084
477.151	14430.2	1.5	224004.9	0.5	0.041	0.044*	0.051
477.779	11444.1	3.5	220744.9	2.5	0.211	0.247	0.166
479.981	24828.5	2.5	233168.5	2.5	0.049	0.051*	0.030**
482.493	14678.3	4.5	221932.2	4.5	0.012	0.020*	0.009**
486.120	0.0	1.5	205711.8	1.5	0.038	0.037*	0.043
487.005	22919.6	3.5	228256.2	3.5	0.127	0.116*	0.101

487.180	11444.1	3.5	216704.6	3.5	0.247	0.234	0.196
487.241	6397.4	2.5	211634.7	1.5	0.054	0.068	0.035
487.643	14430.2	1.5	219500.4	1.5	0.049	0.065*	0.042
487.767	22919.6	3.5	227935.6	2.5	0.309	0.283	0.225
487.916	11444.1	3.5	216397.1	2.5	0.163	0.164	0.170
488.470	0.0	1.5	204720.9	2.5	0.023	0.027*	0.028**
489.648	24028.4	4.5	228256.2	3.5	0.459	0.429	0.215
490.375	11444.1	3.5	215369.6	4.5	0.206	0.193	0.153
491.577	24828.5	2.5	228256.2	3.5	0.174	0.176	0.125**
492.275	28859.8	0.5	231998.6	1.5	0.095	0.096*	0.074
492.355	24828.5	2.5	227935.6	2.5	0.096	0.097*	0.113
492.775	14430.2	1.5	217361.9	1.5	0.029	0.056*	0.027
492.857	22919.6	3.5	225818.9	3.5	0.096	0.127*	0.071
494.335	24028.4	4.5	226320.5	5.5	0.289	0.246	0.228
494.985	14678.3	4.5	216704.6	3.5	0.547	0.566*	0.527
495.131	14430.2	1.5	216397.1	2.5	0.129	0.139	0.137
495.562	24028.4	4.5	225818.9	3.5	0.116	0.191*	0.341
497.635	6397.4	2.5	207349.5	1.5	0.162	0.151*	0.057
497.671	6397.4	2.5	207333.9	2.5	0.114	0.112	0.135
498.279	14678.3	4.5	215369.6	4.5	0.496	0.567	0.660
498.536	16772.4	0.5	217361.9	1.5	0.083	0.094	0.064
499.892	27894.0	1.5	227935.6	2.5	0.116	0.128*	0.137
500.108	14430.2	1.5	214387.4	2.5	0.103	0.062*	0.090
500.511	6397.4	2.5	206193.4	3.5	0.141	0.167	0.027
502.478	22919.6	3.5	221932.2	4.5	0.078	0.108	0.047
503.144	34417.8	2.5	233168.5	2.5	0.187	0.210*	0.090
504.230	6397.4	2.5	204720.9	2.5	0.029	0.050*	0.025
504.684	0.0	1.5	198144.3	0.5	0.262	0.253	0.099**
505.302	24028.4	4.5	221932.2	4.5	0.162	0.180*	0.094
505.501	22919.6	3.5	220744.9	2.5	0.056	0.082*	0.056
506.123	34417.8	2.5	231998.6	1.5	0.157	0.190*	0.147
508.462	6397.4	2.5	203069.9	3.5	0.188	0.147	0.228
509.134	40202.6	1.5	236614.5	0.5	0.038	0.084*	0.033
509.800	0.0	1.5	196152.8	2.5	0.050	0.050*	0.010
509.914	27894.0	1.5	224004.9	0.5	0.507	0.538	0.524
510.425	24828.5	2.5	220744.9	2.5	0.123	0.168	0.137
510.492	11444.1	3.5	207333.9	2.5	0.312	0.382	0.423
510.947	0.0	1.5	195716.1	1.5	0.130	0.131	0.184
511.593	14678.3	4.5	210146.1	5.5	0.758	0.667	0.749
512.354	14678.3	4.5	209856.0	3.5	0.414	0.462*	0.805
512.442	28859.8	0.5	224004.9	0.5	0.061	0.062	0.108

512.534	11444.1	3.5	206555.3	4.5	0.035	0.031*	0.074
513.482	11444.1	3.5	206193.4	3.5	0.588	0.683	0.319
513.684	24828.5	2.5	219500.4	1.5	0.137	0.123	0.135
514.766	0.0	1.5	194263.2	1.5	0.071	0.087*	0.104**
515.025	32155.8	5.5	226320.5	5.5	3.680	3.780	3.759
516.033	22919.6	3.5	216704.6	3.5	0.081	0.083*	0.053
516.617	39600.8	2.5	233168.5	2.5	0.978	0.998	1.224
516.749	34417.8	2.5	227935.6	2.5	0.503	0.532	0.666
516.858	22919.6	3.5	216397.1	2.5	0.078	0.119	0.093
517.396	11444.1	3.5	204720.9	2.5	0.082	0.039*	0.146**
518.539	27894.0	1.5	220744.9	2.5	0.183	0.152*	0.141
518.885	40447.0	3.5	233168.5	2.5	0.105	0.113*	0.031
519.756	39600.8	2.5	231998.6	1.5	0.299	0.339	0.289
520.051	59910.8	1.5	252203.4	1.5	0.294	0.265	0.227
520.597	0.0	1.5	192087.9	0.5	0.239	0.227	0.282
521.169	14678.3	4.5	206555.3	4.5	0.925	0.848	0.580
521.386	40202.6	1.5	231998.6	1.5	0.933	0.756	0.746
521.858	11444.1	3.5	203069.9	3.5	0.343	0.250	0.593
522.008	24828.5	2.5	216397.1	2.5	1.520	1.590	1.560
522.152	0.0	1.5	191516.9	2.5	0.158	0.147	0.156
522.282	22919.6	3.5	214387.4	2.5	0.268	0.246	0.239
522.466	34417.8	2.5	225818.9	3.5	0.244	0.248	0.263
522.631	24028.4	4.5	215369.6	4.5	0.424	0.524	0.297**
522.911	37019.4	4.5	228256.2	3.5	0.876	1.360	1.264
523.020	61005.3	2.5	252203.4	1.5	1.960	1.880	1.819
523.232	28859.8	0.5	219979.0	0.5	0.099	0.071*	0.048
523.595	0.0	1.5	190987.8	1.5	0.099	0.071*	0.126
524.721	16772.4	0.5	207349.5	1.5	0.072	0.059*	0.090
525.512	14430.2	1.5	204720.9	2.5	0.262	0.252	0.279
526.939	32155.8	5.5	221932.2	4.5	0.841	0.559	1.437
526.999	6397.4	2.5	196152.8	2.5	0.038	0.101*	0.0003
528.211	6397.4	2.5	195716.1	1.5	1.060	1.280	0.907
529.270	16772.4	0.5	205711.8	1.5	0.132	0.117	0.120
529.661	37019.4	4.5	225818.9	3.5	7.410	6.770	6.104
530.070	39600.8	2.5	228256.2	3.5	0.074	0.087*	0.078
530.507	28859.8	0.5	217361.9	1.5	0.024	0.015*	0.017**
530.811	14678.3	4.5	203069.9	3.5	0.501	0.339	0.241
530.969	39600.8	2.5	227935.6	2.5	0.472	0.476	0.230
532.296	6397.4	2.5	194263.2	1.5	1.060	0.858	1.045
532.456	40447.0	3.5	228256.2	3.5	1.630	1.490	1.794
532.675	40202.6	1.5	227935.6	2.5	0.254	0.259	0.179**

533.093	14678.3	4.5	202263.2	4.5	1.920	1.830	2.568
533.367	40447.0	3.5	227935.6	2.5	0.654	0.710	0.849
535.179	0.0	1.5	186854.0	0.5	1.240	1.210	1.448
535.318	24828.5	2.5	211634.7	1.5	1.950	1.800	1.887
536.215	27894.0	1.5	214387.4	2.5	0.236	0.269	0.289**
536.691	34417.8	2.5	220744.9	2.5	0.098	0.050*	0.143
537.011	39600.8	2.5	225818.9	3.5	0.023	0.019*	0.018
537.119	6397.4	2.5	192575.6	3.5	0.151	0.159	0.203
537.294	24028.4	4.5	210146.1	5.5	0.217	0.197	0.140**
538.138	24028.4	4.5	209856.0	3.5	6.290	6.080	6.008
538.532	11444.1	3.5	197134.0	3.5	0.459	0.570	0.406
539.465	40447.0	3.5	225818.9	3.5	0.093	0.210	0.123
540.191	6397.4	2.5	191516.9	2.5	1.560	1.330	1.583
540.457	24828.5	2.5	209856.0	3.5	0.280	0.205	0.271
540.795	37019.4	4.5	221932.2	4.5	4.350	4.350	3.921
541.393	11444.1	3.5	196152.8	2.5	4.690	4.280	4.746
541.741	6397.4	2.5	190987.8	1.5	1.170	1.010	1.529
542.260	22919.6	3.5	207333.9	2.5	4.840	4.810	4.262
542.911	27894.0	1.5	212086.5	0.5	0.486	0.480	0.544
543.383	0.0	1.5	184033.0	2.5	0.211	0.195	0.256
544.063	40202.6	1.5	224004.9	0.5	0.427	0.502	0.242
544.249	27894.0	1.5	211634.7	1.5	0.028	0.047*	0.008
544.324	14430.2	1.5	198144.3	0.5	0.172	0.153	0.117
544.555	22919.6	3.5	206555.3	4.5	0.160	0.088*	0.198
545.629	22919.6	3.5	206193.4	3.5	0.147	0.265	0.138
545.771	28859.8	0.5	212086.5	0.5	0.859	0.812	0.781
545.809	32155.8	5.5	215369.6	4.5	11.100	10.030	10.048
546.616	34417.8	2.5	217361.9	1.5	2.110	2.140	1.978
547.126	28859.8	0.5	211634.7	1.5	0.112	0.124	0.104
547.863	24028.4	4.5	206555.3	4.5	3.710	3.340	3.974
548.078	14678.3	4.5	197134.0	3.5	5.150	4.870	4.651
548.589	34417.8	2.5	216704.6	3.5	0.346	0.318	0.229
548.954	24028.4	4.5	206193.4	3.5	2.290	1.820	1.889
549.515	34417.8	2.5	216397.1	2.5	0.189	0.274	0.276
550.051	22919.6	3.5	204720.9	2.5	0.410	0.113*	0.827
550.291	14430.2	1.5	196152.8	2.5	0.160	0.112*	0.058
551.011	40447.0	3.5	221932.2	4.5	0.604	0.448	0.470
551.358	16772.4	0.5	198144.3	0.5	0.675	0.638	0.632
551.616	14430.2	1.5	195716.1	1.5	0.801	0.530	1.020
552.086	11444.1	3.5	192575.6	3.5	3.200	2.870	3.444
552.843	24828.5	2.5	205711.8	1.5	0.396	0.271	0.316

553.893	40202.6	1.5	220744.9	2.5	0.635	0.569	0.484
554.642	40447.0	3.5	220744.9	2.5	6.130	2.860	3.099
555.091	22919.6	3.5	203069.9	3.5	3.530	3.270	3.614
555.333	11444.1	3.5	191516.9	2.5	0.117	0.242	0.014**
555.652	34417.8	2.5	214387.4	2.5	1.820	1.410	1.336
555.870	39600.8	2.5	219500.4	1.5	2.580	2.450	2.650
556.072	14430.2	1.5	194263.2	1.5	1.150	1.160	0.785
556.247	40202.6	1.5	219979.0	0.5	1.240	1.070	1.429
556.528	37019.4	4.5	216704.6	3.5	1.100	0.961	1.503
557.245	27894.0	1.5	207349.5	1.5	1.340	1.240	1.061
557.294	11444.1	3.5	190882.5	4.5	0.900	0.808	0.954
557.590	22919.6	3.5	202263.2	4.5	0.303	0.261	0.165
557.732	40202.6	1.5	219500.4	1.5	0.254	0.268	0.206
558.528	24028.4	4.5	203069.9	3.5	0.094	0.261*	0.095
558.833	16772.4	0.5	195716.1	1.5	0.608	0.468	0.523
560.257	28859.8	0.5	207349.5	1.5	0.513	0.455	0.537
560.695	37019.4	4.5	215369.6	4.5	0.698	0.487	0.885
561.057	24028.4	4.5	202263.2	4.5	0.179	0.254	0.080
561.828	32155.8	5.5	210146.1	5.5	0.310	0.322	0.249
562.123	14678.3	4.5	192575.6	3.5	0.652	0.808	0.682
562.374	27894.0	1.5	205711.8	1.5	1.400	1.160	1.523
562.550	39600.8	2.5	217361.9	1.5	0.877	0.761	0.641
562.880	14430.2	1.5	192087.9	0.5	0.752	0.762	0.866
562.950	6397.4	2.5	184033.0	2.5	2.000	1.900	2.145
563.407	16772.4	0.5	194263.2	1.5	0.293	0.222	0.408
564.282	34417.8	2.5	211634.7	1.5	0.068	0.055	0.112
564.465	40202.6	1.5	217361.9	1.5	0.397	0.343	0.425
564.695	14430.2	1.5	191516.9	2.5	0.209	0.230	0.303
565.448	28859.8	0.5	205711.8	1.5	0.696	0.667	0.628
565.524	27894.0	1.5	204720.9	2.5	0.881	0.764	0.782
565.625	39600.8	2.5	216397.1	2.5	0.021	0.014*	0.012**
565.919	59910.8	1.5	236614.5	0.5	1.780	1.660	1.729
566.387	14430.2	1.5	190987.8	1.5	0.343	0.301	0.367
567.352	40447.0	3.5	216704.6	3.5	1.920	1.930	1.631
567.522	14678.3	4.5	190882.5	4.5	2.580	2.360	2.380
567.916	6397.4	2.5	182479.5	3.5	0.853	0.757	0.858
568.343	40447.0	3.5	216397.1	2.5	0.127	0.203	0.173
568.698	0.0	1.5	175839.8	1.5	2.420	2.230	2.477
570.000	34417.8	2.5	209856.0	3.5	0.550	0.449	0.443
570.398	16772.4	0.5	192087.9	0.5	0.077	0.092	0.076
571.674	40447.0	3.5	215369.6	4.5	0.221	0.105*	0.071

572.123	39600.8	2.5	214387.4	2.5	0.127	0.138	0.064
573.395	32155.8	5.5	206555.3	4.5	1.590	1.900	1.534
574.005	16772.4	0.5	190987.8	1.5	0.567	0.628	0.510
574.102	40202.6	1.5	214387.4	2.5	0.648	0.668	0.743
574.909	40447.0	3.5	214387.4	2.5	0.743	0.614	0.423
577.176	59910.8	1.5	233168.5	2.5	0.611	0.514	0.701
577.256	22919.6	3.5	196152.8	2.5	0.532	0.548	0.768
577.615	37019.4	4.5	210146.1	5.5	0.060	0.061	0.050**
577.679	24028.4	4.5	197134.0	3.5	0.505	0.591	1.002
578.313	34417.8	2.5	207333.9	2.5	0.300	0.220	0.404
578.587	37019.4	4.5	209856.0	3.5	0.038	0.067*	0.125
579.963	14430.2	1.5	186854.0	0.5	0.029	0.040*	0.036
580.367	24828.5	2.5	197134.0	3.5	0.437	0.267	0.387
580.846	61005.3	2.5	233168.5	2.5	1.640	1.590	1.346
581.097	59910.8	1.5	231998.6	1.5	0.548	0.469	0.475
581.288	39600.8	2.5	211634.7	1.5	0.050	0.050*	0.040
582.154	34417.8	2.5	206193.4	3.5	0.565	0.513	0.657
583.320	40202.6	1.5	211634.7	1.5	0.042	0.038*	0.051
583.687	24828.5	2.5	196152.8	2.5	0.291	0.234	0.286
583.789	34417.8	2.5	205711.8	1.5	0.584	0.548	0.670
584.673	11444.1	3.5	182479.5	3.5	0.231	0.176	0.190
584.818	61005.3	2.5	231998.6	1.5	1.500	1.270	1.351
585.178	24828.5	2.5	195716.1	1.5	0.620	0.452	0.581
586.602	0.0	1.5	170473.6	2.5	0.549	0.506	0.554
587.188	34417.8	2.5	204720.9	2.5	0.152	0.165	0.072
587.361	39600.8	2.5	209856.0	3.5	0.121	0.055*	0.113
587.866	32155.8	5.5	202263.2	4.5	0.022	0.046*	0.038
587.954	16772.4	0.5	186854.0	0.5	0.122	0.091	0.140
589.432	22919.6	3.5	192575.6	3.5	0.037	0.044*	0.056
589.611	14430.2	1.5	184033.0	2.5	0.925	0.867	0.923
590.172	6397.4	2.5	175839.8	1.5	0.014	0.008*	0.015**
590.286	40447.0	3.5	209856.0	3.5	0.111	0.065*	0.094
591.104	37019.4	4.5	206193.4	3.5	0.368	0.305*	0.503
593.126	22919.6	3.5	191516.9	2.5	0.049	0.093*	0.021
595.148	59910.8	1.5	227935.6	2.5	0.705	0.620	0.498
595.942	14678.3	4.5	182479.5	3.5	0.343	0.373	0.320
596.136	24828.5	2.5	192575.6	3.5	1.090	1.010	1.056
596.188	39600.8	2.5	207333.9	2.5	0.575	0.577	0.473
597.903	61005.3	2.5	228256.2	3.5	1.260	1.140	1.182
599.206	40447.0	3.5	207333.9	2.5	0.192	0.163	0.275
599.325	24028.4	4.5	190882.5	4.5	0.028	0.037*	0.100

599.927	24828.5	2.5	191516.9	2.5	0.031	0.040	0.013
600.264	39600.8	2.5	206193.4	3.5	0.249	0.114	0.477
601.066	27894.0	1.5	194263.2	1.5	0.047	0.042*	0.050
601.826	24828.5	2.5	190987.8	1.5	0.045	0.042*	0.033
602.006	39600.8	2.5	205711.8	1.5	0.060	0.059	0.042
602.225	37019.4	4.5	203069.9	3.5	0.027	0.056*	0.014
603.331	40447.0	3.5	206193.4	3.5	0.317	0.318	0.309
604.200	40202.6	1.5	205711.8	1.5	0.031	0.023*	0.031
604.580	28859.8	0.5	194263.2	1.5	0.051	0.058	0.071
605.160	37019.4	4.5	202263.2	4.5	0.035	0.024*	0.059
606.743	61005.3	2.5	225818.9	3.5	0.229	0.077*	0.072
607.834	40202.6	1.5	204720.9	2.5	0.345	0.342	0.354
608.738	40447.0	3.5	204720.9	2.5	0.318	0.376	0.254
609.409	59910.8	1.5	224004.9	0.5	0.114	0.082*	0.171
611.164	27894.0	1.5	191516.9	2.5	0.083	0.081	0.090
611.734	39600.8	2.5	203069.9	3.5	0.721	0.696	0.377
612.637	28859.8	0.5	192087.9	0.5	0.076	0.066	0.102
614.914	40447.0	3.5	203069.9	3.5	0.022	0.020*	0.014**
616.793	28859.8	0.5	190987.8	1.5	0.114	0.102	0.138
617.982	40447.0	3.5	202263.2	4.5	0.161	0.145	0.121**
619.542	14430.2	1.5	175839.8	1.5	0.150	0.141	0.174
621.766	59910.8	1.5	220744.9	2.5	0.173	0.140	0.090
624.732	59910.8	1.5	219979.0	0.5	0.151	0.154	0.090
626.020	61005.3	2.5	220744.9	2.5	0.299	0.249	0.278
626.604	59910.8	1.5	219500.4	1.5	0.190	0.162	0.140
626.728	22919.6	3.5	182479.5	3.5	0.057	0.051	0.063
628.126	24828.5	2.5	184033.0	2.5	0.096	0.094	0.103
628.665	16772.4	0.5	175839.8	1.5	0.049	0.043	0.060
628.813	11444.1	3.5	170473.6	2.5	0.018	0.017*	0.019
630.014	32155.8	5.5	190882.5	4.5	0.199	0.261	0.325
630.939	61005.3	2.5	219500.4	1.5	0.089	0.074*	0.096
631.109	24028.4	4.5	182479.5	3.5	0.087	0.111	0.165
632.927	28859.8	0.5	186854.0	0.5	0.027	0.027	0.033
634.307	24828.5	2.5	182479.5	3.5	0.009	0.012	0.011
634.787	39600.8	2.5	197134.0	3.5	0.043	0.046	0.050**
635.136	59910.8	1.5	217361.9	1.5	0.024	0.031*	0.038
636.534	34417.8	2.5	191516.9	2.5	0.043	0.034*	0.047
638.219	40447.0	3.5	197134.0	3.5	0.100	0.074	0.114
638.698	34417.8	2.5	190987.8	1.5	0.070	0.066	0.087
638.764	39600.8	2.5	196152.8	2.5	0.175	0.167	0.170
639.568	61005.3	2.5	217361.9	1.5	0.034	0.032*	0.039

640.549	39600.8	2.5	195716.1	1.5	0.124	0.138	0.156
640.848	14430.2	1.5	170473.6	2.5	0.052	0.052	0.063
646.570	39600.8	2.5	194263.2	1.5	0.023	0.029*	0.016
647.344	59910.8	1.5	214387.4	2.5	0.016	0.012*	0.012
649.097	40202.6	1.5	194263.2	1.5	0.006	0.004*	0.004
649.931	37019.4	4.5	190882.5	4.5	0.078	0.074*	0.085
658.393	40202.6	1.5	192087.9	0.5	0.040	0.039	0.055
661.943	40447.0	3.5	191516.9	2.5	0.009	0.014*	0.008
664.738	40447.0	3.5	190882.5	4.5	0.048	0.041	0.043**
668.385	34417.8	2.5	184033.0	2.5	0.046	0.040*	0.058
675.399	34417.8	2.5	182479.5	3.5	0.019	0.015*	0.017**
686.606	24828.5	2.5	170473.6	2.5	0.005	0.005*	0.005
695.257	40202.6	1.5	184033.0	2.5	0.011	0.011*	0.015
696.443	40447.0	3.5	184033.0	2.5	0.016	0.011*	0.016
701.360	27894.0	1.5	170473.6	2.5	0.029	0.026	0.032
704.066	40447.0	3.5	182479.5	3.5	0.031	0.031	0.037
764.104	39600.8	2.5	170473.6	2.5	0.025	0.023	0.028
823.207	61005.3	2.5	182479.5	3.5	0.007	0.007*	0.006
940.059	100973.9	2.5	207349.5	1.5	0.342	0.262	0.337
944.741	108538.4	3.5	214387.4	2.5	0.258	0.194	0.259
958.446	123600.5	3.5	227935.6	2.5	0.500	0.302	0.420
975.001	114140.1	2.5	216704.6	3.5	0.192	0.134	0.129
977.922	114140.1	2.5	216397.1	2.5	0.236	0.175	0.190
984.931	115173.8	4.5	216704.6	3.5	0.512	0.354	0.426
986.987	108538.4	3.5	209856.0	3.5	0.389	0.362	0.388
997.955	97940.4	1.5	198144.3	0.5	0.585	0.423	0.515
998.040	115173.8	4.5	215369.6	4.5	1.040	0.870	1.066
998.213	132989.9	3.5	233168.5	2.5	1.580	1.030	1.661
1012.199	108538.4	3.5	207333.9	2.5	0.143	0.157	0.113
1018.199	97940.4	1.5	196152.8	2.5	0.457	0.388	0.343
1018.614	138441.2	1.5	236614.5	0.5	0.166	0.119	0.141
1020.229	108538.4	3.5	206555.3	4.5	0.759	0.632	0.324
1021.475	118499.8	1.5	216397.1	2.5	1.360	0.894	1.236
1024.015	108538.4	3.5	206193.4	3.5	0.306	0.282	0.053
1026.422	123318.6	1.5	220744.9	2.5	0.583	0.392	0.589
1026.617	130849.6	4.5	228256.2	3.5	1.120	0.729	1.187
1028.050	114363.2	0.5	211634.7	1.5	0.792	0.561	0.769
1029.397	123600.5	3.5	220744.9	2.5	0.714	0.394	0.478
1034.565	123318.6	1.5	219979.0	0.5	0.253	0.179	0.237
1035.410	131676.2	2.5	228256.2	3.5	0.573	0.268	0.333
1038.184	97940.4	1.5	194263.2	1.5	0.838	0.617	0.833

1038.864	131676.2	2.5	227935.6	2.5	0.662	0.419	0.630
1039.709	123318.6	1.5	219500.0	1.5	0.203	0.076	0.051
1039.943	100973.9	2.5	197134.0	3.5	1.500	1.140	1.435**
1047.439	130849.6	4.5	226320.5	5.5	3.760	2.580	3.576**
1049.695	132989.9	3.5	228256.2	3.5	0.833	0.688	0.945
1050.652	100973.9	2.5	196152.8	2.5	0.568	0.469	0.507
1052.939	115173.8	4.5	210146.1	5.5	3.670	2.670	3.612**
1053.231	132989.9	3.5	227935.6	2.5	0.276	0.188	0.167
1054.694	157388.9	0.5	252203.4	1.5	1.190	0.801	1.177
1055.665	138441.2	1.5	233168.5	2.5	0.327	0.180	0.200
1056.151	115173.8	4.5	209856.0	3.5	0.345	0.247	0.403
1057.849	108538.4	3.5	203069.9	3.5	0.483	0.264	0.726
1062.219	131676.2	2.5	225818.9	3.5	1.730	1.390	1.944**
1063.333	123318.6	1.5	217361.9	1.5	0.733	0.461	0.742
1066.956	108538.4	3.5	202263.2	4.5	1.890	1.310	2.232**
1068.531	118499.8	1.5	212086.5	0.5	0.335	0.240	0.333
1068.647	97940.4	1.5	191516.9	2.5	0.382	0.230	0.477**
1068.864	138441.2	1.5	231998.6	1.5	1.140	0.655	1.028
1071.936	100973.9	2.5	194263.2	1.5	0.138	0.085	0.126
1072.848	114140.1	2.5	207349.5	1.5	0.603	0.406	0.569
1074.069	123600.5	3.5	216704.6	3.5	0.471	0.388	0.436
1075.424	114363.2	0.5	207349.5	1.5	0.102	0.084	0.102
1077.246	132989.9	3.5	225818.9	3.5	0.501	0.279	0.341
1086.336	114140.1	2.5	206193.4	3.5	1.030	0.742	0.605**
1089.694	123600.5	3.5	215369.6	4.5	1.510	1.030	1.418**
1094.314	115173.8	4.5	206555.3	4.5	0.490	0.329	0.482
1098.083	123318.6	1.5	214387.4	2.5	0.276	0.202	0.231
1098.651	115173.8	4.5	206193.4	3.5	0.012	0.011*	0.019
1101.487	123600.5	3.5	214387.4	2.5	0.517	0.352	0.578
1103.982	114140.1	2.5	204720.9	2.5	0.366	0.186	0.482
1104.445	100973.9	2.5	191516.9	2.5	0.237	0.126	0.316
1117.393	138441.2	1.5	227935.6	2.5	0.387	0.267	0.478
1122.731	131676.2	2.5	220744.9	2.5	0.343	0.235	0.414
1124.334	132989.9	3.5	221932.2	4.5	1.320	0.942	1.365**
1124.487	114140.1	2.5	203069.9	3.5	0.146	0.069	0.532**
1126.533	123318.6	1.5	212086.5	0.5	0.119	0.091	0.126
1141.380	108538.4	3.5	196152.8	2.5	0.103	0.052	0.140
1183.150	130849.6	4.5	215369.6	4.5	0.146	0.107	0.132
1213.899	132989.9	3.5	215369.6	4.5	0.218	0.082	0.192**
1214.431	108538.4	3.5	190882.5	4.5	0.242	0.195	0.330**
1226.917	100973.9	2.5	182479.5	3.5	0.416	0.325	0.487**

1262.213	157388.9	0.5	236614.5	0.5	0.239	0.153	0.255**
1283.719	97940.4	1.5	175839.8	1.5	0.181	0.126	0.197
1291.962	115173.8	4.5	192575.6	3.5	0.747	0.569	0.818
1292.383	114140.1	2.5	191516.9	2.5	0.117	0.082	0.133
1320.854	115173.8	4.5	190882.5	4.5	0.774	0.572	0.861
1324.610	108538.4	3.5	184033.0	2.5	0.516	0.391	0.565
1350.694	131676.2	2.5	205711.8	1.5	0.416	0.323	0.471
1352.428	108538.4	3.5	182479.5	3.5	0.472	0.342	0.501
1366.055	132989.9	3.5	206193.4	3.5	0.162	0.088	0.315
1378.678	97940.4	1.5	170473.6	2.5	0.451	0.345	0.501**
1381.265	123318.6	1.5	195716.1	1.5	0.100	0.070	0.088
1426.942	132989.9	3.5	203069.9	3.5	0.205	0.215	0.148
1430.758	114140.1	2.5	184033.0	2.5	0.180	0.128	0.193
1443.568	132989.9	3.5	202263.2	4.5	0.085	0.073	0.028**
1449.783	123600.5	3.5	192575.6	3.5	0.253	0.196	0.262
1451.520	138441.2	1.5	207333.9	2.5	0.111	0.060	0.162**
1463.294	114140.1	2.5	182479.5	3.5	0.216	0.157	0.216**
1466.297	123318.6	1.5	191516.9	2.5	0.114	0.097	0.113**
1486.275	123600.5	3.5	190882.5	4.5	0.357	0.252	0.346**

¹ Experimental wavelengths from [5]. ² Experimental energy levels from [5,6]. ³ Calculated transition probabilities from [5]. ⁴ Calculated transition probabilities obtained in the present work. gA -values with * symbol correspond to transitions for which $CF < 0.05$ in HFR+CPOL calculations while gA -values with ** symbol correspond to transitions for which $dT > 0.25$ in MCDHF calculations (see text).

A first observation that can be made when looking at this table is that our HFR+CPOL transition probabilities are in good agreement with the results previously published by Raassen *et al.* [5], with a mean ratio $gA_{\text{HFR+CPOL}}/gA_{\text{Raassen}}$ equal to 0.95 ± 0.21 (where the number after $\pm$ represents the standard deviation from the mean), which is quite comparable to the ratio we get when comparing our HFR calculations with and without core polarization corrections, i.e. $gA_{\text{HFR+CPOL}}/gA_{\text{HFR}} = 0.98 \pm 0.10$.

It is also interesting to note that the agreement between the HFR+CPOL and MCDHF results obtained in the present work is generally good, the mean ratio between both sets of data, $gA_{\text{HFR+CPOL}}/gA_{\text{MCDHF}}$, being equal to 1.08 ± 0.48 , if we exclude the two transitions at 526.999 and 555.333 Å for which the gA -values differ from each other by one or two orders of magnitude. This means that the majority of our gA -values calculated using the two methods agree within a few tens of percent. Such a comparison is shown in Figure 1 where transition probabilities obtained using the HFR+CPOL approach are plotted against those deduced from MCDHF calculations.

The quality of the transition probabilities obtained in our work can also be estimated from parameters such as the cancellation factor (CF) and the uncertainty parameter (dT) for HFR+CPOL and MCDHF calculations, respectively. As a reminder, the former parameter is defined by [7]:

$$CF = \frac{\left[\sum \sum y_{\beta J}^{\gamma} \langle \beta J \| P^{(1)} \| \beta' J' \rangle y_{\beta' J'}^{\gamma'} \right]^2}{\sum \sum \left| y_{\beta J}^{\gamma} \langle \beta J \| P^{(1)} \| \beta' J' \rangle \right| \left| y_{\beta' J'}^{\gamma'} \right|} \quad (1)$$

where $P^{(1)}$ is the dipole operator for the transition between two atomic states $|\gamma J\rangle$ and $|\gamma' J'\rangle$ developed in terms of pure basis states $|\beta J\rangle$ and $|\beta' J'\rangle$, with $y_{\beta J}^{\gamma}$ and $y_{\beta' J'}^{\gamma'}$ as mixing coefficients, respectively. According to Cowan [7], very small values of this parameter (typically $CF < 0.05$) may be expected to show significant errors in the computed line strengths. In our work, it was verified that the CF -values

were larger than 0.05 for most of the lines listed in Table 2, the only exceptions occurring for 91 transitions (among 367) generally characterized by rather weak gA -values (typically smaller than 10^9 s^{-1}). This is illustrated in Figure 2 where the CF parameter is plotted as a function of HFR+CPOL transition probabilities for all Os VI lines considered in the present work.

As for the dT parameter, it is expressed by [16]:

$$dT = \frac{|A_B - A_C|}{\max(A_B, A_C)} \quad (2)$$

where A_B and A_C are transition probabilities in Babushkin (length) and Coulomb (velocity) gauges, the electric dipole transition moment having the same value in both formalisms for exact solutions of the Dirac equation [17]. The dT parameter thus provides a statistical estimate of the uncertainty of MCDHF transition rates for approximate solutions for which the transition moment differs from one gauge to another. For transitions listed in Table 2, the average value of dT was found to be equal to 0.17 ± 0.06 , which means that the uncertainties affecting most of our MCDHF gA -values do not exceed 25%. The few exceptions for which the dT parameter was found to be greater than 25% concern only 42 transitions out of the 367 listed in Table 2. This is illustrated in Figure 3 where dT is plotted as a function of gA_{MCDHF} .

Finally, it should be noted that, if we set aside the transitions listed in Table 2 for which, both $CF < 0.05$ (in the HFR+CPOL calculations) and $dT > 0.25$ (in the MCDHF calculations), there remain 250 transitions whose differences between the gA -values obtained using the two methods do not exceed 30%, the mean relative deviation $DgA/\langle gA \rangle$ (where $DgA = |gA_{\text{HFR+CPOL}} - gA_{\text{MCDHF}}|$ and $\langle gA \rangle = (gA_{\text{HFR+CPOL}} + gA_{\text{MCDHF}})/2$) being equal to 0.29. Consequently, at least for these 250 lines, the uncertainty on the HFR+CPOL and MCDHF transition probabilities obtained in our work can be estimated at most 30%, the gA -values of other transitions can be affected by slightly larger uncertainties up to a factor of two.

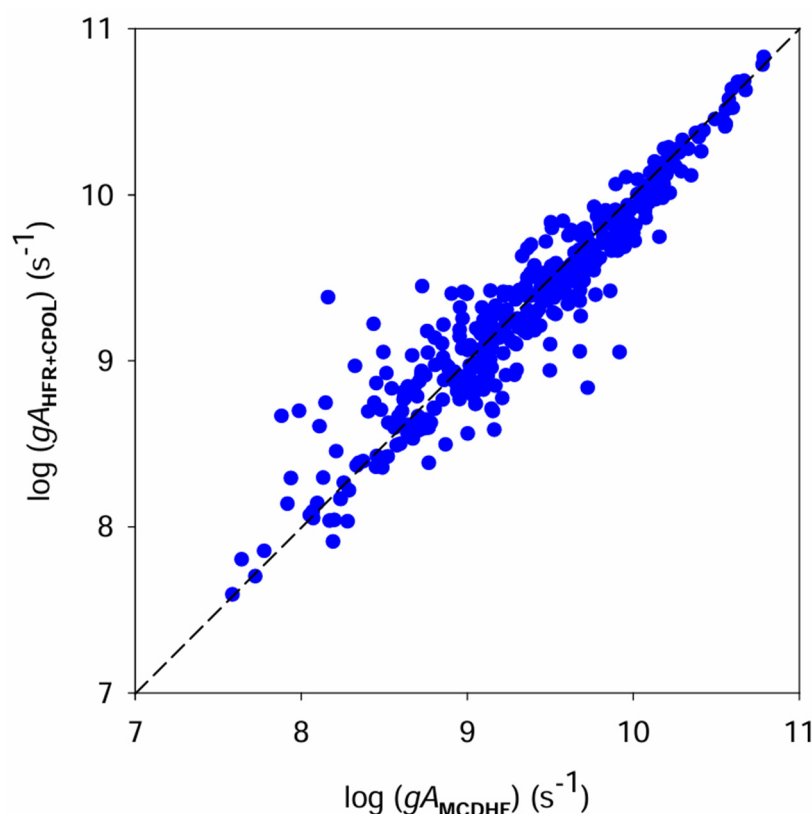


Figure 1. Comparison between transition probabilities (gA) obtained using the HFR+CPOL method and those deduced from MCDHF calculations.

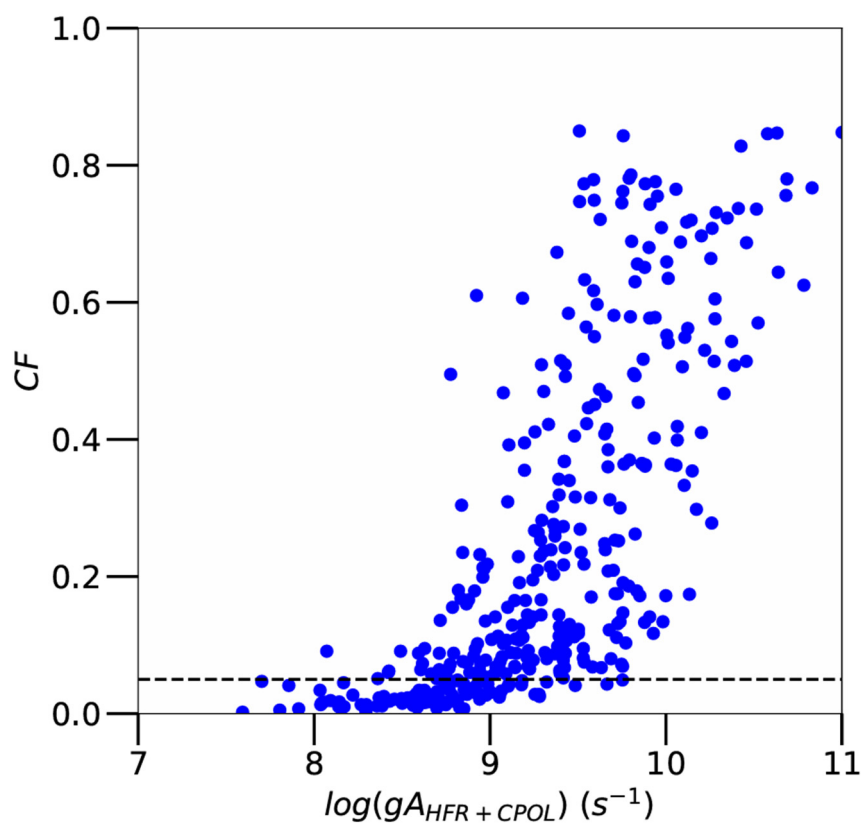


Figure 2. Cancellation factors (CF) as a function of gA -values obtained using the HFR+CPOL method for Os VI transitions. The dotted line corresponds to $CF = 0.05$.

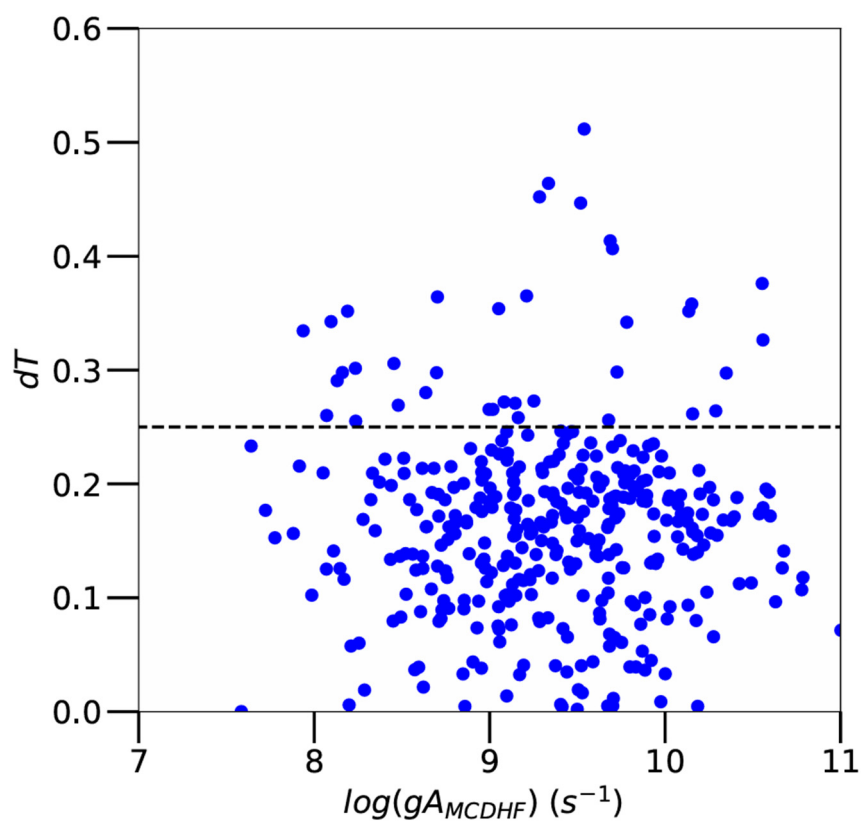


Figure 3. Uncertainty parameter (dT) as a function of gA -values obtained using the MCDHF method for Os VI transitions. The dotted line corresponds to $dT = 0.25$.

4. Conclusions

New transition probabilities for experimentally observed lines in the Os VI spectrum are reported in the present work. They were obtained using two different computational approaches based on the pseudo-relativistic Hartree-Fock method including core-polarization corrections (HFR+CPOL) and the fully relativistic Multiconfiguration Dirac-Hartree-Fock method (MCDHF). Based on the detailed comparison showing a good agreement between the two sets of results (within a few tens of percent for most transitions), it can be concluded that the gA -values reported in this paper are the most reliable currently available for the Os VI ion. These new atomic data will be useful for the analysis of the spectra emitted by fusion plasmas produced in Tokamaks such as ITER.

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