Transitions among low-lying levels of Mg V

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Abstract. We have undertaken a large-scale Breit-Pauli configuration interaction calculation of transitions among lower-lying levels in Mg V. We optimised orbitals to represent the main configurations (including the LS-dependency of the states under consideration) together with all the major correlation effects. All one- and two-electron replacements from a basic reference comprising the dominant configurations were allowed for in the calculation. A small selection of oscillator strengths and transition rates is presented here. We focus in this short report on transitions with the lower state dominated by the 2\(p^4\) configuration. Our results agree closely with the calculations of Fischer but differ markedly from the recent work of Bhatia et al.

1. Introduction

Mg V is an important ion in the oxygen-isoelectronic sequence. Its lines are detected in the planetary nebula NGC 7027 [1-4] and in wide spectral ranges from soft X-rays to the ultraviolet region. They are also expected to be seen in the solar and other astrophysical plasmas. Only a few calculations are available for the atomic structure of Mg V. Fischer and Saha [5] presented multiconfiguration Dirac-Hartree-Fock (MCDHF) energy levels belonging to the ground configuration 2\(s^2p^3\) \((^3P, ^1D, ^1S)\) and E2 and M1 transitions among these levels for some oxygen-like ions including Mg V. Tachiev and Fischer [6] later presented data for E1, E2, M1, M2 transitions from odd levels belonging to 2\(s^2p^5\), 2\(s^22p^33s\) and 2\(s^22p^33d\) configurations of Mg V. The personal web-page of Fischer [7] also presents both \textit{ab initio} and energy adjusted values for E1 transitions among all but one of the levels belonging to the above configurations and the even configuration 2\(s^22p^33p\), although the level 2\(s^22p^3(2P^o)3d^1D\) was missing in these tabulations. Recently, Bhatia, Landi and Eissner [8] reported a calculation of atomic structure and collisional data for Mg V. They [8] compared their 6-, 9-, and 24-configuration calculated values of 86 fine-structure levels with the observed values as given by the NIST [9] database. It might be expected that the 24-configuration results would be more accurate than the two other sets. However, on many occasions, their 6-configuration energy levels show better agreement with the observed values. For example their 6-configuration results \(^3P_{0,1,2}\) levels belonging to the configuration 2\(s^22p^3(2P)3s\) are some 800 cm\(^{-1}\) lower than corresponding observed values whereas their 24-configuration results are about 14,000 cm\(^{-1}\) lower than corresponding observed values. Similar behaviour is manifested for the levels of 2\(s^22p^3(2P)3d^3P\) configuration. For 2\(s^22p^3(2P)3p\)\(^3P\) the observed values are not available. For this case too their 24-configuration energy values differ by amounts similar to their 6-configuration results. Interestingly, their 6-configuration result for the 2\(p^6\) \(^1S_0\) pushed the level at least six positions down. In short their energy levels of the 6-configuration or 24-configuration cases show some erratic behaviour and in such a case both atomic and scattering data could be in error. It is for this reason we wanted to investigate this ion using our
superposition of configurations code CIV3 [10]. The details of the theoretical methods can be found elsewhere and will not be presented here.

2. Calculation Method
The 1s and 2s functions are those given by Clementi and Roetti [11] for the Mg V Hartree-Fock (HF) ground state. We then reoptimised the HF 2p function and also optimised a 3s function on the $2p^3(2D^o)3s^3D^o$ energy. The 3p and 3d functions are optimised as spectroscopic orbitals on the energies of the lowest $2p^33p^1P$ and $2p^33d^3D^o$ states, using this same 2p. It is important to take a balanced account of correlation across the range of states under consideration, as well as allowing for an LS dependency on the optimal orbitals. For example, the optimal 3p for $2p^33p$ for $3D$ symmetry will be slightly different from that optimised on the $1P$ state. Additional orbitals were therefore optimised to allow for these differences and to account for the effects of electron correlation not included within the Hartree-Fock or single-configuration approximation. As an example, the 4s orbital was taken as correlation type and optimised on the lowest energy of \{2s^22p^4 + 2s^22p^2ns ms\} $^1S$ with $3 \leq n, m \leq 5$. The remaining two s-orbitals were also optimised to account for other correlation effects. The 4p and 5p functions were optimised on the energies of $2p^33p^1P$ and $3D$ respectively including all configurations of the form $2p^3(2D, 2P)np^1P$ and $2p^3(2D, 2P)np^3D$, with $n = 3, 4$ and $m = 3, 4, 5$. These two functions therefore act as corrections to 3p orbital. The 6p function, on the other hand, was chosen to be of correlation type and optimised on the ground state using configurations of the form \{2s^22p^4 + 2s^22p^2np mp\} $^3P$ with $3 \leq n, m \leq 6$. The 4d and 6d functions were taken as correction orbitals and were optimised on the lowest of $2p^3(S, 2D, 2P)np^3D^o$ while 5d functions optimised on \{2s^22p^4 + 2s^22p^4nd\} $^3P$ to account for correlation effects in the $n = 2$ shell. Similarly the remaining orbitals i.e. 7p, 8p, 7d, 8d, 4f, 5f and 5g are optimised as either correction or correlation type.

Our initial set of configurations was generated by allowing all one- and two- and some three-electron promotions from the main configurations labelling the states of interest, using all the available orbitals, but retaining a closed 1s$^2$ shell in all configurations. This process resulted in a total of 380,559 configuration state functions (CSFs) for the 9 even parity symmetries and 12 odd parity symmetries. In order to reduce the scale of the calculation, we formed a truncated set of CSFs by deleting those whose eigenvector strengths were less than 0.001 in every eigenvector in which they were involved. The effect of this truncation on either the energy values or the CI coefficients of the CSFs which remained was minimal. With this truncated set of CSFs, we formed the configuration set for each J-value : 0-4 for even parity, 0-5 for odd parity. In total, this gave us 120,736 CSFs. The Hamiltonian for this calculation was composed of the Schrödinger Hamiltonian augmented by the Breit-Pauli operators: spin-orbit, spin-other-orbit, spin-spin, the mass correction and Darwin terms. Finally, when the \textit{ab initio} Hamiltonians for each J-value were obtained, we made small adjustments to the diagonal matrix elements so that the eigenvalue differences were close (within a few cm$^{-1}$) to the corresponding experimental values.

3. Results and Discussion
In Table 1 we present a sample of our 15 fine-structure compared with other available results. Notice that both the present energies and those of Fischer [7] are fine-tuned while those of Bhatia \textit{et al} [8] are \textit{ab initio}. Both the present and those of Fischer [7] agree with the measurements [9] within few cm$^{-1}$ while those of Bhatia \textit{et al} [8] show large disagreement both in values and in energy ordering.
Table 1. Present fine-tuned energies are compared with NIST\cite{9} energies and those of Bhatia \textit{et al} \cite{8} and Fischer \cite{7}. All energy differences are in cm$^{-1}$.

| Index | Configuration | Term | \text{[8]} | \text{[7]} | Present | NIST \cite{9} |
|-------|---------------|------|----------|----------|---------|-------------|
| 1     | 2s$^2$2p$^4$  | $^3$P$_2$ | 0.00     | 0.00     | 0.00    | 0.00       |
| 2     | 2s$^2$2p$^4$  | $^3$P$_1$ | 1902     | 1778.5   | 1783.1  | 1783.10    |
| 3     | 2s$^2$2p$^4$  | $^3$P$_0$ | 2690     | 2507.0   | 2521.8  | 2521.80    |
| 4     | 2s$^2$2p$^4$  | $^1$D$_2$ | 39208    | 35927.8  | 35926.9 | 35926.00   |
| 5     | 2s$^2$2p$^4$  | $^1$S$_0$ | 77893    | 77279.5  | 77279.9 | 77279.00   |
| 6     | 2s2p$^5$     | $^3$P$_2$ | 29368    | 283223.3 | 283210.3 | 283212.30  |
| 7     | 2s2p$^5$     | $^3$P$_1$ | 295395   | 284834.2 | 284826.6 | 284828.80  |
| 8     | 2s2p$^5$     | $^3$P$_0$ | 296319   | 285713.2 | 285711.7 | 285712.00  |
| 9     | 2s2p$^5$     | $^1$P$_1$ | 418585   | 397489.6 | 397480.5 | 397482.00  |
| 10    | 2p$^6$       | $^1$S$_0$ | 700201   | 662970.5 | 662971.1 | 662970.00  |
| 11    | 2s$^2$2p$^3$(4S$^o$)3s | $^3$S$_1$ | 672683 | 684540.8 | 684541.2 | 684541.00 |
| 12    | 2s$^2$2p$^3$(2D$^o$)3s | $^3$D$_3$ | 717781 | 727774.5 | 727774.2 | 727774.00 |
| 13    | 2s$^2$2p$^3$(2D$^o$)3s | $^3$D$_3$ | 717986 | 727775.8 | 727776.3 | 727776.00 |
| 14    | 2s$^2$2p$^3$(2D$^o$)3s | $^3$D$_3$ | 717648 | 727779.9 | 727782.7 | 727782.00 |

Table 2. Comparison of some Mg V oscillator strengths for spin-allowed transitions.

| Lower level | Upper level | $\lambda$(Å) | This work | \text{[7]} | \text{[8]} |
|-------------|-------------|---------------|-----------|-----------|-----------|
| $2p^4$ $^3$P$_2$ | $2s2p^5$ $^3$P$_2$ | 353.092 | 0.1176 | 0.1188 | 0.1179 | 0.1459 |
| $^3$P$_1$ | 351.088 | 0.0395 | 0.0398 | 0.0396 | 0.0490 |
| $^3$P$_0$ | 353.329 | 0.0648 | 0.0650 | 0.0650 | 0.0806 |
| $^3$P$_1$ | 353.300 | 0.0392 | 0.0396 | 0.0393 | 0.0486 |
| $^3$P$_0$ | 352.201 | 0.0525 | 0.0529 | 0.0526 | 0.0651 |
| $^3$P$_1$ | 354.223 | 0.1562 | 0.1579 | 0.1566 | 0.1943 |
| $2p^4$ $^3$P$_2$ | $2p^3$(4S$^o$)3s $^3$S$_1$ | 146.083 | 0.0522 | 0.0518 | 0.0517 | 0.0678 |
| $^3$P$_1$ | 146.465 | 0.0510 | 0.0506 | 0.0504 | 0.0647 |
| $^3$P$_0$ | 146.623 | 0.0508 | 0.0504 | 0.0503 | 0.0667 |
| $2p^4$ $^3$P$_2$ | $2p^3$(2D$^o$)3s $^3$D$_3$ | 137.411 | 0.0612 | 0.0621 | 0.0618 | 0.0684 |
| $^3$D$_2$ | 137.407 | 0.0130 | 0.0132 | 0.0130 | 0.0140 |
| $^3$D$_2$ | 137.745 | 0.0514 | 0.0521 | 0.0519 | 0.0586 |
| $^3$D$_1$ | 137.741 | 0.0195 | 0.0198 | 0.0196 | 0.0217 |
| $2p^4$ $^3$P$_0$ | $2p^3$(4S$^o$)3d $^3$D$_3$ | 137.881 | 0.0683 | 0.0693 | 0.0690 | 0.0783 |
| $^3$D$_2$ | 121.645 | 0.2220 | 0.2179 | 0.2230 | 0.2890 |
| $^3$D$_2$ | 121.656 | 0.0402 | 0.0395 | 0.0403 | 0.0522 |
| $^3$D$_1$ | 121.921 | 0.1934 | 0.1900 | 0.1945 | 0.2538 |
| $^3$D$_1$ | 121.923 | 0.0653 | 0.0641 | 0.0655 | 0.0854 |
| $^3$P$_0$ | 122.033 | 0.2580 | 0.2534 | 0.2590 | 0.3388 |

In Table 2 we compare our oscillator strengths in length ($f_L$) and velocity ($f_V$) gauges with the corresponding results of Fischer \cite{7} and most recent calculation of Bhatia \textit{et al} \cite{8}, for
transitions with one of the $2p^4$ levels as the lower level.

The present results and those of Fischer [7] agree very well, but deviate significantly from the recent calculations of Bhatia et al [8] which are consistently higher, by up to almost 45%.

Table 3. Mg V radiative rates ($A_L$, in s$^{-1}$) for some selected strong transitions.

| Lower level | Upper level | $\lambda$(Å) | This work | [9]       | [7]       |
|-------------|-------------|--------------|-----------|-----------|-----------|
| $2p^4$ $^3P_2$ | $2s2p^5$ $^3P_2$ | 353.092      | 6.29(09)† | 6.12(09) | 6.31(09) |
| $2p^4$ $^3P_1$ | $2s2p^5$ $^3P_2$ | 351.088      | 3.57(09)  | 3.46(09) | 3.57(09) |
| $2p^4$ $^3P_1$ | $2s2p^5$ $^3P_1$ | 353.300      | 2.09(09)  | 2.04(09) | 2.09(09) |
| $2p^4$ $^3P_0$ | $2s2p^5$ $^3P_0$ | 352.201      | 8.47(09)  | 8.23(09) | 8.49(09) |
| $2p^4$ $^1D_2$ | $2s2p^5$ $^1P_1$ | 276.582      | 3.13(10)  | 3.12(10) | 3.14(10) |
| $2p^4$ $^1S_0$ | $2s2p^5$ $^1P_1$ | 312.302      | 1.83(09)  | 1.89(09) | 1.84(09) |
| $2s2p^5$ $^1P_1$ | $2p^5$ $^1S_0$ | 376.665      | 2.26(10)  | 2.20(10) | 2.25(10) |

†: power of 10 in parentheses

In Table 3, we present a comparison of transition rates ($A$-values) of transitions selected on the basis of the highest accuracy ratings ($B^+$) given in [9]. There is excellent agreement between our results and those of Fischer [7]. This agreement between independent calculations suggests that our results may represent an improvement in accuracy over the ones given in [9]. We checked the $A$-values of Bhatia et al [8] only for the $B^+$- rated transitions and found their results to be 30-40% higher than those we have calculated in the present work. Hence their values are not included in the comparison in Table 3.

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