

Mo VI $J=3/2, 5/2$ Energy Levels, Oscillator Strengths and Landé g -values

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Abstract.

Relativistic configuration interaction calculations have been done for Mo VI $4p^5 4d^2 J = 5/2$ and $nf^2 F_{5/2}$ ($n=4-6$) wave functions. Level energies and E1 oscillator strengths for transitions between these states and the $nd^2 D$ ($n=4-6$) states have been obtained. The calculated LS compositions of all 11 levels of $4p^5 4d^2 J = 5/2$ have been found to be in good agreement with other designations. While most calculated level energies agree well with the most recent experimental work, large discrepancies in a few (upper) levels do exist. The oscillator strength of all 84 transitions are computed, and 36 of the largest ($f > 0.001$) are presented here. Most of the oscillator strengths are computed for the first time.

1. Introduction

Mo VI is a member of the Rb I isoelectronic sequence with $4p^6 4d$ as its ground state configuration. It's important for diagnostics of controlled fusion plasmas.

Our interest in this species came about from our work on Mo V [1], where we calculated the positions of the $4p^5 4d^3$ levels. These levels were interpenetrating the $4d(np+4f)$, $5s5p$ levels. The changing core ($4p^5$ vs $4p^6$) population means fewer correlation effects nearly cancel, thus requiring the use of much more extensive wave functions. It was suggested [2] that Mo VI might offer a test of our methods, as it was simpler (fewer electrons) and that some results were available for the $4p^5 4d^2$ levels.

The investigation of Mo VI began in the early 1930's. So far, the one-electron spectra of Mo VI have been extensively studied, but study of the core-excited states such as the $4p^5 4d^2$ and $4p^5 4d 5s$ states have gained much less attention. It's been established that the $4p^5 4d^2$ states are strong perturbers of the nf and np one-electron spectra, and they are responsible for an important part of Mo VI's spectrum. However, identifying them experimentally is not an easy task. For example, identification of the $4p^6 4d - 4p^5 4d^2$ transitions is complicated by three facts [3]. First, there are other transitions in Mo VI that lie in the same spectral region. Second, there are transitions in Mo V that behave very similarly to the transitions of interest. Finally, there is strong interaction between the $4p^6 nf$ states and the $4p^5 4d^2$ states. In 1985, Tauheed *et al* measured the energy values of $4p^5 4d^2$ for the first time and established 38 out of the total 45 levels [4]. In 1991, Kancerevicius *et al* [3] published their results for Mo VI,

giving energy values of 37 out of 45 levels of $4p^5 4d^2$ (some of them are available on the NIST database [5]) and 20 out of 23 levels of $4p^5 4d 5s$. For the $J=5/2$ levels of $4p^5 4d^2$, the differences between Tauheed *et al* and Kancerevicius *et al* are sometimes large, varying from 0 to 6300 cm^{-1} and are not in one direction.

The strong interaction between $4p^6 nf$ and $4p^5 4d^2$ also complicates the computations for their level energies. Before this work, there was only one semi-empirical computation by Cowan for these levels. The results were not formally published, but they can be derived from [4]. Comparing with [3], his calculated levels are too high by 972 to 7772 cm^{-1} .

These large discrepancies, while illustrating the elusiveness of the $4p^5 4d^2$ levels, provided motivations to the present calculation and one on-going experiment work [2]. In our work, we have done relativistic configuration interaction calculations for energy values of Mo VI $4p^6 nd$ ($n=4-6$) even parity states, $4p^6 nf$ ($n=4-6$) and $4p^5 4d^2 J=5/2$ odd parity states, and oscillator strengths of transitions between them. To simplify notations, we will drop the closed core in the one-electron configurations from now on. We will also use “Rn” to denote the levels of $4p^5 4d^2$ with the lowest one being R1.

2. Methodology

The methodology employed is the Relativistic Configuration Interaction (RCI) [6] method. Since the relativistic effects and correlation effects are not additive, they are treated simultaneously by RCI. The Hamiltonian is the Dirac-Coulomb(-Breit) one. The many-electron correlation effects are incorporated as in a first-order wave function. Since J and parity are good quantum numbers, RCI calculations for each J , parity set are independent of one another. Considerable efficiencies are achieved by recognizing that for many properties, such as transition matrix elements, the major accuracy criterion is the relative spacing of levels achieved within the set. The position of one set of levels relative to another set can be left to determination by experiment.

In the present instance, it was decided to focus on the $J=5/2$ (odd) levels, as those from $4p^5 4d^2$ have a very strong interaction with the $4p^6 nf$ Rydberg series. While the $J=7/2$ (odd) levels also have a strong interaction with this series, calculation of just the one series took several calendar months (“off and on”), restricting us to doing less than all the J , parity sets associated with the $4p^5 4d^2$ configuration. While there is some commonality of one-electron (radial) and N-electron (configurations used) basis sets between $J=5/2$ (odd) and $7/2$ (odd), which would reduce the time element for a $J=7/2$ (odd) calculation, the $J=1/2$ (odd) and $3/2$ (odd) $4p^5 4d^2$ levels interact (less) strongly with the $4p^6 np$ Rydberg series, which is, *a priori*, *terra incognita* to RCI.

The even parity levels were selected by looking for those levels which could have large f -values with (some) $J=5/2$ (odd) levels. Our choice was the $4p^6 nd$ series ($J=3/2$ and $5/2$). These series have no strong perturbers, and determining the relative positions of the levels within a RCI calculation is a relatively simple affair, as it is not necessary

to include much core-valence correlation, as we had to do for $J=5/2$ (odd). This does mean that RCI energy differences between $J=5/2$ (odd) and $J=3/2$ ($J=5/2$) are not accurate, thus requiring the use of an experimental value.

The reference space is chosen first. All configurations corresponding to the levels of interest are included. Their radial functions are generated by numerically solving the Dirac-Fock (DF) equations using Desclaux's code [7]. A common set of DF radials are used for a given parity's state. The first-order wave function is constructed by making single and double excitations from the reference space. For those originally unoccupied subshells, i.e. virtuals, the radial functions are represented by Relativistic Screened Hydrogenic (RSH) functions. For each symmetry l , usually 3 RSH functions are adequate to represent the compact portion of the entire Rydberg and the continuum series of the radial space. The only adjustable parameter in the RSH function is the effective charge, Z^* . Starting with an estimate, its value is determined by minimizing the appropriate root during the energy variation process.

Once the approximate wave function is obtained, it's straightforward to calculate the atomic properties such as the electric dipole oscillator strength (or f -values). All transitions are calculated using our "one-pass" algorithm [9, 10] which computes all transitions simultaneously for a fixed energy difference, and then scales appropriately the individual f -values with the experimental energy difference when available.

Because the even and odd parity wave functions are computed with separate basis sets, non-orthonormality effect must be included when computing the f -values. This is done using the method of King *et al* [11]. Details of the methodology can be found in [12].

3. Calculations

3.1. Mo VI nf ($n=4-6$) + $4p^5 4d^2$ $J=5/2$ odd parity states

In the beginning, we included only nf ($n=4-6$), $4p^5 4d^2$ in the reference space because of the strong interactions between them. Later, when we found the nearby higher states of $4p^5 4d 5s$ and $7f$ had a relatively large composition in the wave function, we enlarged the reference space by including these two configurations. However, they are less correlated than other configurations in the reference space due to restrictions on the size of basis set.

The DF calculation for $4f^2 F_{5/2}$ yields the numerical radial functions of the closed core: $1s, \dots, 4p$ and $4f$. Other radials are obtained from the DF calculations for the corresponding reference configurations, with the $4d$ radials taken from $4p^5 4d^2$ R1 $J=5/2$.

Three sets of virtuals with $l \leq 4$ have been used. The exception is $l=5$, which has only one RSH function. The $4d, 4f$ and $4p$ electrons are treated as valence ones. Since the $\langle r \rangle$ of $4f$ is about 1 a.u. larger than that of $4d$ and $4p$, to capture the diffuse portion of the whole Rydberg series, we put some restrictions on the kind of correlation

configurations used when calculating the first set of virtuals. That is, though we make single and double excitations from 4p, 4d and 4f in nf and $4p^5 4d^2$, we leave out those double excitations from 4p which need much larger Z^* 's. The second set of virtuals is added by making double excitations from 4p. Since the $\langle r \rangle$ of the 4s and 4p radials are very close, excitations involving 4s should need similar Z^* 's as those from 4p. Finally, the third set of virtuals is added to saturate all the important correlations.

Due to the limitation on the RCI matrix size (20k), we don't include $l > 5$ in the virtual space. To estimate their correlation effect on the energy values of $4p^5 4d^2$, we extrapolate the energy contributions from double excitations of $4p^2$ in 4f, 4p4d in $4p^5 4d^2$. The extrapolated correlation energy from $4p^2 \rightarrow vl^2$ ($l > 5$), $vl v(l+2)$ (v denotes virtual subshells, $l \geq 4$) is roughly about 76 meV in 4f, one-third of which will contribute to increase the energy of the $4p^5 4d^2$ levels relative to the 4f level. The extrapolated energy of $4p4d \rightarrow vl v(l+1)$ ($l \geq 5$) is about 51 meV, which will decrease the energy of the $4p^5 4d^2$ levels with respect to the 4f level. Thus the estimated contribution from $l > 5$ is about 26 meV, which if included, will decrease the energy of the $4p^5 4d^2$ levels by about 26 meV. However, there are still other smaller contributions such as double excitations of 4s4p, whose inclusion will add more correlation energy to the 4f level and thus make the energy of the $4p^5 4d^2$ states higher. Therefore, the total net effect from $l > 5$ should be less than 26 meV. So we don't include these extrapolations in our final results.

Some second-order effects are found to be important to the level energies. During the calculation, we notice $4p^5 4d vd$ has both a large energy contribution and a large weighted coefficient in the upper $4p^5 4d^2$ levels. However, it's not explicitly correlated as the reference configurations are. We estimate the effect of correlating it on the energy values by decreasing its energy difference relative to the 4f level in the corresponding diagonal energy matrix element by 4 eV. This results in the $4p^5 4d^2$ R11 level being lowered by $\sim 720 \text{ cm}^{-1}$, the $4p^5 4d^2$ R10 level being lowered by $\sim 290 \text{ cm}^{-1}$. Then we introduce almost all big excitations (with correlation energy $> 40 \text{ meV}$) in $4p^5 4d^2$ to $4p^5 4d vd$. As a result, the total correlation energy in $4p^5 4d vd$ is increased by 1.820 eV. The $4p^5 4d^2$ R11 and R10 level are lowered by 842 cm^{-1} and 413 cm^{-1} respectively with respect to the 4f level.

There are also other second-order effects that are important. The largest of these should come from products of the largest pair excitations (quadruple excitations) and the products of the largest single and pair excitations (triple excitations). Among the correlation excitations, the most differentially large ones are double excitation of $4p^2 \rightarrow 4d^2$, single excitations of $4p \rightarrow 4f, 5f, vf$ and $4s \rightarrow 4d$. We combine these together to have $4p^4 \rightarrow 4d^4$, $4p^3 \rightarrow 4d^2 f$, $4s 4p^2 \rightarrow 4d^3$ and introduce them to the reference configurations. The net effect is biggest on the $4p^5 4d^2$ R11 level, which is lowered by 951 cm^{-1} . The $4p^5 4d^2$ R10 level is lowered by 306 cm^{-1} . Impacts on the remaining levels are small.

With the large reference space and large number of second-order effects, the basis set grows rapidly and would be 8 times the 20k limit. The bulk of it is due to correlations

in $4p^5 4d^2$ and $4p^5 4d$ *vd*. To make sure all the reference configurations are correlated equivalently, some methods must be taken to reduce the basis size. The one that has been extensively used in this work is REDUCE [13]. Briefly, this rotates the original basis functions for a correlation configuration to maximize the number of basis functions having a zero interaction with all the reference functions. These “zero interactions” are then discarded. We have applied REDUCE to about 300 configurations. The final RCI matrix size is 19,621.

3.2. Mo VI nd ($n=4-6$) even parity states

The reference space consists of the 3 levels of interest to us: 4d, 5d and 6d. The numerical DF radial functions for 1s, ..., 4p and 4d are generated from the DF calculation for 4d, while the 5d and 6d radials are from the separate DF calculation for 5d and 6d. All these calculations are done using Desclaux’s code [7].

Three sets of virtuals with $l \leq 5$ are used. The virtuals are added in “layers” as in the odd parity case. The first set is for excitations from the outermost orbital 4d, 5d and 6d. The second set, in addition to the first set, is introduced to represent excitations from the shallow core orbital 4p and 4s. Finally, the third set of virtuals is added to saturate those differentially important configurations.

4. Results and Analysis

4.1. Mo VI $nf + 4p^5 4d^2$ $J=5/2$ odd parity states

Though the $4p^5 4d^2$ levels are not LS pure, to compare with experiments, we use the LS coupling scheme to analyze them. The results for the LS composition percentage of all 11 levels and comparison with other designations are shown in table 1. In each LS term, the one inside the parenthesis is the LS term of $4d^2$. The interaction between the nf one-electron states and the $4p^5 4d^2$ states are most obvious in the R10 (see table 1) and 5f levels. In these two levels, the percentage of $4p^5 4d^2$ and 5f are very close with the leading composition accounting for slightly more than 50%. As can be seen from the table, we are in good agreement with both Cowan’s calculations [4] and Kancerevicius’s results. The exception is the R10 level where the composition percentages differ a lot among the three sets of data. The difference between RCI and Kancerevicius *et al* may be due to the different choice of the reference configurations. In RCI, if we designate that the R10 level has only $4p^5 4d^2$ and 5f, no 4f component, the percentage of $4p^5 4d^2$ (1G) 2F and 5f would be 25% and 47%, quite close to Kancerevicius’s result of 24% and 43%. However, RCI also calculates 27% from $4p^5 4d^2$ (3F) 2F which is missing in Kancerevicius *et al*’s result.

The general good agreement in composition percentage doesn’t necessarily mean good agreement in energy values. The RCI results for energy values are shown in table 2, along with the experimental values. According to the statement in [8], one will expect that Tauheed’s data to be less reliable. It may be interesting to note that except

for $4p^5 4d^2$ R10 and 5f, for each level, the RCI result agrees well with at least one experiment. For all the levels except R10 and R11, we are in good agreement with Kancerevicius *et al* with the average absolute difference being 455 cm^{-1} . As for the R11 level, the RCI value is 6668 cm^{-1} too high comparing with Kancerevicius *et al*, but only 810 cm^{-1} too high comparing with Tauheed *et al*. The RCI level value for R10 lies almost the midway between the two experiments with the difference being about 3000 cm^{-1} .

The large “error” in $4p^5 4d^2$ R10 and R11 suggests there might be some missing correlation or radial deficiency in them. To locate the possible reasons, we begin with examining the DF radial space. Separate DF calculations for $4p^5 4d^2$ R1 and R11 using Desclaux’s code [7] show the energy difference between them is $153\,486 \text{ cm}^{-1}$. In a separate RCI calculation for $4p^5 4d^2$ using the DF radials taken from the $4p^5 4d^2$ R1 level, at the DF level, the energy difference is $160\,472 \text{ cm}^{-1}$. So there is a big error of about 7000 cm^{-1} due to using a common set of radial functions. This shows that the 4d radials are indeed quite different between the top and the bottom level. To compensate for this difference, we add $4d \rightarrow vd$, the symmetry preserving single excitation, to the basis set. Then the energy difference becomes $153\,359 \text{ cm}^{-1}$, very close to that calculated using Desclaux’s code. We are thus assured that as long as $4d \rightarrow vd$ is present, the difference among the 4d radials of the $4p^5 4d^2$ levels should be adequately compensated. The next question arises is: how different are the radials of the core (including 4p) in $4p^5 4d^2$ from those in 4f? To test this, we take the DF radials of 1s, ..., 4p from the 4f state and attach to them the 4d radials from $4p^5 4d^2$ R1. Using these radial functions, we run RCI for $4p^5 4d^2$. At the DF level, the total energy of R1 is off by only 644 cm^{-1} . A similar test has been taken for $4p^5 4d^2$ R11 and there the R11 level is off by 179 cm^{-1} from using the core radials of the 4f state. These indicate that except for the outmost 4d and 4f orbital, the inner orbitals are similar between the 4f and $4p^5 4d^2$ states. Moreover, to make up this small difference between the 4f and $4p^5 4d^2$ state, we have included the symmetry preserving single excitation $4s \rightarrow vs$ and $4p \rightarrow vp$ in the basis set.

To find possible missing correlations in $4p^5 4d^2$, we have done separate RCI calculations for $4p^5 4d^2 J=5/2$ only and compared the energy contribution from each configuration to that in the big RCI run. There are several configurations that exhibit energy loss, with the maximum to be 28%. Among them is $4p^5 f^2$ (f^2 denotes either two DF f subshells, or two virtual f subshells, or combination of both). It has a total energy contribution of 144 meV in the separate run, but 103 meV in the big run. This energy loss can be understood from perturbation theory where the second-order energy is given by:

$$-\frac{|H_{0,i}|^2}{|H_{0,0} - H_{i,i}|} \quad (1)$$

Since the $4p^5 4d^2$ levels are more preferentially correlated, the energy difference between $4p^5 4d^2$ and $4p^5 vf^2$ (i.e. the denominator) is increased, resulting in a decreased energy

contribution. Sometimes the energy loss can be partially recovered by adding those big excitations to the problem configuration. We estimate the impact of correlating $4p^5 v f^2$ by decreasing the denominator by 3 eV (the total correlation energy in $4p^5 4d^2$ R1 level is about 6.5 eV). This helps gain back only 3 meV in the correlation energy. For other configurations that show energy loss, we have made up a portion of the missing energy by adding additional virtuals.

Close to the final stage, we include the magnetic Breit operator in the Hamiltonian. Its impact on the energy values is large, especially on those of the upper levels. The levels are brought down by 130–674 cm^{-1} relative to the 4f level except 6f which is increased by 77 cm^{-1} . The upper $4p^5 4d^2$ levels are thus improved, while the lower ones differ even more from the experiments. We have also estimated the retardation and radiative effects using the second version of Desclaux’s code [15]. Differentially, they don’t exceed 93 cm^{-1} and 52 cm^{-1} respectively, so small that we have neglected them.

4.2. Mo VI nd ($n=4-6$) even parity states

The RCI level energies are shown in table 3.

The magnetic Breit effect is examined at the final stage of calculation. For the $J=3/2$ states, the 5d and 6d level is lowered by 60 cm^{-1} and 86 cm^{-1} relative to the 4d level. The effect on the $J=5/2$ states is even smaller. Therefore, we have neglected the magnetic Breit effect in table 3.

For the $J=3/2$ states, the average absolute error in energy difference is 459 cm^{-1} . Though this looks a little big considering the one-electron configurations studied, it’s actually a small number comparing to the energy value of the 6d level which is 386 167 cm^{-1} [5]. Indeed, the average percent error between adjacent levels is only 0.43%. For the $J=5/2$ states, the average absolute error is 383 cm^{-1} , while the average percent error between adjacent levels is 0.39%. The small separation error indicates that the RCI basis functions are accurately “mixed together”.

For both of the J states, the differentially most important excitations are pair excitations from $4p nd$ and single excitations from $4p$ and $4s$.

4.3. Mo VI Oscillator strengths (f -values)

When calculating the f -values, the energy values measured by Kancerevicius *et al* [3] have been used for transition energies. Transitions having big (> 0.001) f -values are shown in table 4. For transitions $nd \ ^2D_{3/2} \rightarrow nf, 4p^5 4d^2 J=5/2$ ($n=4-6$), there are 28 out of 3×14 big transitions. 22 transitions are included in table 4 with the two gauges agreeing on average to 6.6%. The remaining 6 transitions (6d – $4p^5 4d^2$ R5, R8; 5d – $4p^5 4d^2$ R3, R5, R6, 4f) are left out from the table due to large gauge discrepancies. They involve either double-electron jumps where $4p^5 4d^2$ levels are involved, or a shell jump. We have done some test runs to improve their gauge agreement. For example, we have tried to attach a numerical 5d radial to the radial space of the odd parity states to saturate the radial overlap between the 5d in the even parity state and the d’s in

the odd parity state. While this had a big effect on the gauge agreements of $6d - 4p^5 4d^2$ R10, 5f which were improved by 12% and 9% respectively, those of the above 6 transitions were improved less or even got worse. The largest excluded f -value is 0.167 in Coulomb gauge with the gauge agreement being 27%.

For transitions $nd \ ^2D_{5/2} \rightarrow nf, 4p^5 4d^2 \ J=5/2$ ($n=4-6$), there are 16 out of 3×14 big transitions. Two of them are left out from table 4 due to large gauge discrepancies. For the remaining 14 transitions in table 4, the average gauge agreement is 5.0%.

From table 4, the R11 level is strongly connected only to the 4d level, which may give some difficulty in determining its position during the experiment. As shown in table 1, none of the $4p^5 4d^2$ levels is LS pure except R11. However, some LS selection rules can still be observed in table 4. For example, the f -values of $nd \ ^2D_{3/2} \rightarrow nf \ ^2F_{5/2}$ are much larger than those of $nd \ ^2D_{5/2} \rightarrow nf \ ^2F_{5/2}$, which is expected because the former are the principal lines that satisfy $\Delta J = \Delta L$. For the same reason, the f -value of $4d \ ^2D_{5/2} \rightarrow R11$ is one order of magnitude larger than that of $4d \ ^2D_{3/2} \rightarrow R11$ as the R11 level is about 99% 2D pure. The one-electron-jump transitions from $4d \ ^2D_{3/2}$ to R1, R2, R3 and R7 have very small f -values because their leading term is a quartet which violates the $\Delta S = 0$ rule. The leading term of R6 is also a quartet but the transition involving it has a nontrivial f -value. This is because it has some 2F composition characteristic of the principal line and some 4f composition which has a big matrix element. Although the R4 level has a slightly larger (8%) composition of 2F than the R6 level, it doesn't show up in table 4 because there is almost no 4f composition in it.

As for transitions from 5d or 6d to $4p^5 4d^2$, they involve double-electron jumps and should have been forbidden. But in table 4, they correspond to small but non-zero f -values. This is mainly because the $4p^5 4d^2$ levels are, to a more or less extent, interlaced with the nf one-electron spectra, which are connected to the nd states by electric dipole transitions. This same reason can be applied to account for the larger f -value of transitions involving the $4p^5 4d^2$ R10 level. As can be seen from table 1, the R10 level has totally a 49% nf composition which contributes to its oscillator strengths.

Calculations made by Cowan are also listed in table 4 whenever applicable. While most of the RCI f -values in table 4 are in good agreement with Cowan's (where available), the RCI f -values for $4d \rightarrow 4p^5 4d^2$ R10 are significantly smaller than Cowan's. To understand this, we did single configuration (Dirac-Fock) calculations for the transitions from $4d \ ^2D_{3/2}$ to $4f \ ^2F_{5/2}$ (.98), $5f \ ^2F_{5/2}$ (.15), $6f \ ^2F_{5/2}$ (.046), $4p^5 4d^2$ R10 $J=5/2$ (2.41), and $4p^5 4d \ 5s$ R4 $J=5/2$ (.17). The numbers in parentheses are the f -value in the Babuskin gauge. Comparing to the RCI values in table 4, we argue that oscillator strength has been transferred from (DF) 4f and $4p^5 4d^2$ R10 to (RCI) 5f and 6f. The sums are only roughly conserved (3.59 vs 2.92), but the energy range is quite large, so the theory [17] is likely not as applicable. This argument also presumes that the unavailable 4f, 5f, 6f Cowan f -values are small to moderate in size.

5. Conclusion

We have done relativistic configuration interaction calculations for the nd ($n=4-6$) 2D states and the nf ($n=4-6$) $^2F_{5/2}$, $4p^5 4d^2 J=5/2$ states of Mo VI. The level energies and the oscillator strengths of the electric dipole transitions between these states have been obtained. We have found good agreement with the most recent experimental work by Kancercivius *et al* in the level energies except for the top two levels (R10 and R11) of $4p^5 4d^2 J=5/2$. The situation of these two levels is complicated. In an earlier work by Tauheed *et al*, the $4d - 4p^5 4d^2$ R11 transition was identified and the R11 level was determined. Our RCI result for this level tends to confirm their level value. However, Kancercivius *et al* mentioned in their work that the above identified transition was not found in their spectra and has assigned a much smaller energy value for the R11 level. Kancercivius *et al* has used semi-empirical calculations to help identify the levels. Their reported standard deviation is 268 cm^{-1} which is not trivial. Besides, in their calculations, there was no $4p^5 4d 5d$ in the interacting configuration list which we have found to be important to the R10 and R11 level. Since the $4p^5 4d 5d$ will add more correlation to these two levels, if it had been included in Kancercivius *et al*'s calculation, their level energies would have been even smaller. Given these considerations, the position of the R10 and R11 level still need some future work. Determination of experimental Landé g -value may be helpful in this regard.

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Table 1. Mo VI nf and $4p^5 4d^2 J=5/2$ LS Composition^a

Level	Level Composition (%)
4f	82 4f ² F, 12 (¹ G) ² F, 3 (¹ D) ² F — 86 4f ² F, 11 (¹ G) ² F
5f	56 5f ² F, 25 (³ F) ² F, 13 (¹ G) ² F, 4 (¹ D) ² F — 54 5f ² F, 25 (³ F) ² F
6f	90 6f ² F, 3 (¹ G) ² F — 93 6f ² F, 3 (¹ G) ² F
R1	68 (³ F) ⁴ D, 22 (³ P) ⁴ D, 5 (³ F) ⁴ F, 3 (³ P) ⁴ P 68 (³ F) ⁴ D, 22 (³ P) ⁴ D, 6 (³ F) ⁴ F, 3 (³ P) ⁴ P 68 (³ F) ⁴ D, 22 (³ P) ⁴ D
R2	89 (³ P) ⁴ P, 4 (³ F) ⁴ D, 3(³ F) ⁴ F 86 (³ P) ⁴ P, 5 (³ F) ⁴ D, 3(³ F) ⁴ F 87 (³ P) ⁴ P
R3	38 (³ F) ⁴ G, 21 (³ F) ⁴ F, 16 (³ F) ² F, 11 (¹ G) ² F, 5 (¹ D) ² D, 4 (³ P) ⁴ P 40 (³ F) ⁴ G, 20 (³ F) ⁴ F, 14 (³ F) ² F, 9 (¹ G) ² F, 7 (¹ D) ² D, 4 (³ P) ⁴ P 38 (³ F) ⁴ G, 20 (³ F) ⁴ F
R4	51 (¹ D) ² D, 15 (³ F) ² D, 8 (³ F) ² F, 7 (³ F) ⁴ G, 8 (¹ G) ² F, 5 (³ F) ⁴ F, 4 (¹ D) ² F 52 (¹ D) ² D, 15 (³ F) ² D, 7 (³ F) ² F, 9 (³ F) ⁴ G, 6 (¹ G) ² F, 5 (³ F) ⁴ F, 4 (¹ D) ² F 55 (¹ D) ² D, 15 (³ F) ² D
R5	26 (³ F) ⁴ F, 23 (¹ G) ² F, 18 (³ F) ² F, 13 (¹ D) ² D, 7 (³ P) ⁴ D, 9 (³ F) ⁴ G 29 (³ F) ⁴ F, 21 (¹ G) ² F, 18 (³ F) ² F, 12 (¹ D) ² D, 9 (³ P) ⁴ D, 4 (³ F) ⁴ G 30 (³ F) ⁴ F, 22 (¹ G) ² F
R6	45 (³ F) ⁴ G, 33 (³ F) ⁴ F, 8 (¹ G) ² F, 4 (³ F) ² F, 4 (¹ D) ² D, 3 (³ P) ⁴ D 44 (³ F) ⁴ G, 33 (³ F) ⁴ F, 8 (¹ G) ² F, 5 (³ F) ² F, 4 (¹ D) ² D, 3 (³ P) ⁴ D 45 (³ F) ⁴ G, 30 (³ F) ⁴ F
R7	51 (³ P) ⁴ D, 25 (³ F) ⁴ D, 15 (³ P) ² D, 7 (³ F) ⁴ F 52 (³ P) ⁴ D, 25 (³ F) ⁴ D, 13 (³ P) ² D, 7 (³ F) ⁴ F 50 (³ P) ⁴ D, 26 (³ F) ⁴ D

Level	Level Composition (%)
R8	84 (¹ D) ² F, 5 (³ P) ² D, 5 (³ F) ² D, 3 (¹ D) ² D 82 (¹ D) ² F, 5 (³ P) ² D, 5 (³ F) ² D, 3 (¹ D) ² D 82 (¹ D) ² F
R9	64 (³ P) ² D, 15 (³ P) ⁴ D, 6 (¹ D) ² F, 7 (¹ D) ² D, 5 (³ F) ² D 66 (³ P) ² D, 13 (³ P) ⁴ D, 6 (¹ D) ² F, 6 (¹ D) ² D, 6 (³ F) ² D 65 (³ P) ² D, 15 (³ P) ⁴ D
R10	26 (³ F) ² F, 25 (¹ G) ² F, 46 5f ² F, 3 4f ² F 29 (³ F) ² F, 30 (¹ G) ² F, 36 5f ² F, 3 4f ² F 24 (¹ G) ² F, 43 5f ² F
R11	71 (³ F) ² D, 16 (¹ D) ² D, 12 (³ P) ² D 70 (³ F) ² D, 16 (¹ D) ² D, 12 (³ P) ² D 70 (³ F) ² D, 18 (¹ D) ² D

^a The $4p^5 4d^2$ levels are denoted with Rn . For each level, the first line is from RCI, the second line is from Tauheed *et al* [4] and percentages less than 3% are omitted. The third line for each level is from Kancerevicius *et al* [3] and percentages less than 10% are omitted. Results of RCI have no magnetic Breit effect.

Table 2. Mo VI $J=5/2$ energy levels(cm^{-1}) and Landé g -values^a

Level ^b	RCI ^c	Kancerevicius ^d	Tauheed ^e	Cowan ^f	Landé g^c
4f	0	0	0	0	0.857
4p ⁵ 4d ² R1	20985	21885	24508	25308	1.356
4p ⁵ 4d ² R2	33311	33641	35631	36499	1.554
4p ⁵ 4d ² R3	36021	36133	35955	38621	0.838
4p ⁵ 4d ² R4	41950	42333	43491	44540	1.084
4p ⁵ 4d ² R5	48138	48102	47903	50122	0.967
4p ⁵ 4d ² R6	51177	51473	50326	52406	0.822
4p ⁵ 4d ² R7	63407	62820	61204	63792	1.317
4p ⁵ 4d ² R8	70513	70018	70018	71103	0.912
4p ⁵ 4d ² R9	83005	82233	81234	82424	1.214
5f	99081	98050			0.858
4p ⁵ 4d ² R10	130274	127011	133311	134069	0.859
4p ⁵ 4d ² R11	152422	145754	151612	153526	1.197
6f	169057	169125			0.857

^a All energy values are given with respect to the 4f $^2F_{5/2}$ level. The energy value with respect to the ground state 4d $^2D_{3/2}$ can be found by adding 267048.8 cm^{-1} [5] to each energy entry.

^b The designation of each Rn level is given in table 1.

^c This work, includes the magnetic Breit effect.

^d From [3].

^e From [4].

^f Derived from [4].

Table 3. Mo VI (4d+5d+6d) energy levels (cm^{-1})

Level	J=3/2		J=5/2 ^a	
	RCI ^b	Expt ^c	RCI ^b	Expt ^c
4d	0	0	0	0
5d	282954	282827	281172	281076
6d	385446	386167	383300	383970

^a Energy values for $J=5/2$ are with respect to the 4d $^2D_{5/2}$ state. The energy value with respect to the ground state 4d $^2D_{3/2}$ can be found by adding 2584.3 cm^{-1} [5] to each energy value.

^b This work.

^c From [5].

Table 4. RCI results for Mo VI $nd \rightarrow nf + 4p^5 4d^2 J=5/2$ f -values ($n=4-6$)^a

Transitions	Coulomb Form	Babuskin Form	Spread ^b	Other Values ^c
4d $^2D_{3/2} \rightarrow 4f$	0.2849	0.2896	0.8%	
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R3	0.0087	0.0090	2.1%	
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R5	0.0628	0.0666	2.9%	0.052
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R6	0.0143	0.0155	4.1%	0.020
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R7	0.0023	0.0025	3.2%	
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R8	0.0771	0.0808	2.3%	0.066
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R9	0.0207	0.0221	3.3%	0.016
4d $^2D_{3/2} \rightarrow 5f$	0.4451	0.4835	4.1%	
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R10	1.7480	1.8442	2.7%	2.946
4d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R11	0.1346	0.1404	2.1%	0.136
4d $^2D_{3/2} \rightarrow 6f$	0.2863	0.3061	3.3%	
5d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R7	0.0011	0.0014	15.0%	
5d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R8	0.0417	0.0551	14.0%	
5d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R9	0.0115	0.0140	9.6%	
5d $^2D_{3/2} \rightarrow 5f$	0.6207	0.7048	6.3%	
5d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R10	0.2545	0.2365	3.7%	
5d $^2D_{3/2} \rightarrow 6f$	0.1502	0.1804	9.2%	
6d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R9	0.0041	0.0056	15.0%	
6d $^2D_{3/2} \rightarrow 5f$	0.2091	0.2781	14.0%	
6d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R10	0.2282	0.1853	10.0%	
6d $^2D_{3/2} \rightarrow 4p^5 4d^2$ R11	0.0055	0.0041	15.0%	
6d $^2D_{3/2} \rightarrow 6f$	0.9901	1.0228	1.6%	
4d $^2D_{5/2} \rightarrow 4f$	0.0136	0.0139	1.3%	
4d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R5	0.0082	0.0090	4.4%	
4d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R7	0.0101	0.0109	3.4%	0.010
4d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R8	0.0146	0.0154	2.8%	0.014
4d $^2D_{5/2} \rightarrow 5f$	0.0056	0.0062	4.4%	
4d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R10	0.0256	0.0269	2.6%	0.043
4d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R11	2.1563	2.2486	2.1%	2.883
4d $^2D_{5/2} \rightarrow 6f$	0.0250	0.0268	3.5%	
5d $^2D_{5/2} \rightarrow 5f$	0.0299	0.0337	6.0%	
5d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R10	0.0122	0.0115	3.0%	
5d $^2D_{5/2} \rightarrow 6f$	0.0072	0.0086	9.0%	
6d $^2D_{5/2} \rightarrow 5f$	0.0101	0.0133	14.0%	
6d $^2D_{5/2} \rightarrow 4p^5 4d^2$ R10	0.0107	0.0084	12.0%	
6d $^2D_{5/2} \rightarrow 6f$	0.0479	0.0494	1.6%	

^a RCI f -values include the magnetic Breit effect. Only transitions with $f > 0.001$ are listed.

^b Spread = $\frac{|f_v - f_i|}{f_v + f_i} \times 100\%$.

^c Values are derived from Cowan's calculations in [4].

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