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Spectrum and Energy Levels of Five-Times Ionized Zirconium (Zr VI)

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Abstract

We carried out a new analysis of the spectrum of five-times-ionized zirconium Zr VI. For this we used sliding-spark discharges together with normal- and grazing-incidence spectrographs to observe the spectrum from 160 to 2000 Å. These observations showed that the analysis of this spectrum by Khan Z. A. et al. 1985 *Phys. Scr.* **31** 837 contained a significant number of incorrect energy levels. We have now classified ~420 lines as transitions between 23 even-parity levels 73 odd-parity levels. The $4s^24p^5$, $4s4p^6$, $4s^24p^44d$, $5s$, $5d$, $6s$ configurations are now complete, although a few levels of $4s^24p^45d$ are tentative. We determined Ritz-type wavelengths for ~135 lines from the optimized energy levels. The uncertainties range from 0.0003 to 0.0020 Å. Hartree-Fock calculations and least-squares fits of the energy parameters to the observed levels were used to interpret the observed configurations. Oscillator strengths for all classified lines were calculated with the fitted parameters. The results are compared with values for the level energies, percentage compositions, and transition probabilities from recent *ab initio* theoretical calculations. The ionization energy was revised to $777380 \pm 300 \text{ cm}^{-1}$ ($96.38 \pm 0.04 \text{ eV}$).

1. Introduction

The zirconium atom has atomic number $Z=40$. Five-times-ionized zirconium, Zr VI, is isoelectronic with neutral Br. The ground state is $4s^24p^5\ ^2P$, and excited states are mainly of the type $4s^24p^4nl$. The first work on this spectrum was done by Paul and Rense [1]. From their observation of transitions to the ground term, they determined the $4p^5\ ^2P$ interval as well as the first excited state $4s4p^6\ ^2S_{1/2}$ and several levels of the $4p^44d$ and $4p^45s$ configurations. Subsequently, Chaghtai [2,3] re-observed the resonance transitions and found that nearly all of Paul and Rense's excited levels were in error. Chaghtai gave values for 16 new levels in these configurations. Subsequently, Ekberg, Hansen, and Reader [4] re-investigated the spectrum and gave improved values for nearly all levels of the $4p^44d$ and $5s$ configurations. Seven of Chaghtai's levels were found to be spurious. Chaghtai et al [5] later extended the resonance lines to the $4p^45d$, $6s$, $6d$, and $7s$ configurations. Khan et al [6] determined the levels of the $4p^45p$ configuration by using longer wavelength transitions from the above configurations to levels of $4p^45p$.

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In the present work we re-observed the spectrum of Zr VI in the vacuum ultraviolet and revised the analysis considerably. In particular, 13 of the 21 levels of $4p^45p$ reported by Khan et al [6] were found to be spurious. Several new levels of $4p^44d$, $5s$, $5d$, and $6s$ reported in [6] were also found to be spurious.

2. Experiment

The observations used for this work were the same as used for earlier work in our laboratory on zirconium [7]. The main light source was a low-voltage sliding-spark with metallic Zr electrodes. The source was operated as described by Reader et al [8]. From 500 to 2000 Å the spectra were recorded on our 10.7-m normal-incidence vacuum spectrograph. From 160 to 500 Å the spectra were recorded on our 10.7-m grazing incidence spectrograph. Both instruments had gratings with 1200 lines/mm. The plate factor for the normal-incidence spectrograph was about 0.78 Å/mm. The plate factor for the grazing-incidence spectrograph at 350 Å was 0.25 Å/mm. From 600 to 2000 Å the spectra were calibrated by spectra of Cu II excited in a hollow cathode discharge. Below 600 Å calibration was obtained from lines of Y in various stages of ionization. Shifts between the positions of the reference spectra and those of the unknown spectra due to differing illumination of the spectrograph were removed by use of impurity lines of oxygen, nitrogen, carbon, and silicon. Complete references for the calibration spectra are given in Ref. [7].

Ionization stages were distinguished by comparing the intensities of the lines at various peak currents in the spark. The spectra of Zr VI were relatively enhanced at a peak current of about 2000 A.

The wavelengths, intensities, and classifications of the observed lines of Zr VI are given in table 1. The intensities are estimates of photographic plate blackening. No effort was made to harmonize the intensities through the complete region of observation. The general uncertainty of the wavelengths is ± 0.005 Å. Hazy lines (h) were given an uncertainty of ± 0.010 Å; perturbed (p), or asymmetric lines (s, l) an uncertainty of ± 0.020 ; unresolved (u) or doubly classified (dc) lines an uncertainty of ± 0.030 Å. By *perturbed* we mean that the measured position may possibly be affected by the presence of a close line. The line at 1749.353 Å could not be measured in the original observations because of a local defect in the emulsion of one of the photographic plates. It was later recorded with an image plate [9,10] on the normal-incidence spectrograph. Its wavelength uncertainty was also taken as ± 0.005 Å. All uncertainties are reported at the level of one standard deviation.

3. Spectrum analysis and level value determination

The analysis was carried out in a manner similar to that used for the recent analysis of Mo V [11]. As described there “Interpretation of the spectrum was guided by calculations of the level structures and transition probabilities with the Hartree-Fock code of Cowan [12]. Further guidance was provided by construction of two-dimensional transition arrays with the computer spreadsheet method described by Reader [13].”

The odd parity energy levels are given in table 2, the even levels in table 3. In addition to the usual spectroscopic designations in either LS or jI (pair) coupling, the levels are given

shorthand designations that are used in the classification of the spectral lines. The shorthand designations are explained in the footnotes to tables 2 and 3. As described in [11] “The values of the energy levels were optimized with the computer program ELCALC [14], an iterative procedure in which the observed wave numbers are weighted according to the inverse square of their uncertainties. The uncertainties of the level values given by this procedure are also listed.” For the level optimization only the most reliably classified lines were used. That is, lines that were very weak or that appeared with suspiciously high intensities were excluded.

Figure 1 shows a schematic overview of the positions of the $4s^24p^5$, $4s4p^6$, $4s^24p^44d$, $5s$, $5p$, $5d$, and $6s$, configurations. It also shows the calculated positions of the $4s^24p^44f$ and $4s4p^54d$ configurations, although no levels have as yet been established for them.

3.1 $4s^24p^44d$ levels

Nearly all levels of this configuration that could combine with the ground state were present in [4]. Remaining as unknown were $(^3P)^4D_{1/2,7/2}$, $(^1S)^2D_{5/2}$, $(^3P)^4F_{7/2,9/2}$, $(^3P)^2F_{7/2}$, $(^1D)^2G_{7/2,9/2}$, and $(^1D)^2F_{7/2}$. Values for these 9 levels were given in [6]. Our present work shows that 6 of the 9 were spurious. Details of these 9 levels are:

1. $(^3P)^4D_{1/2}$ – new level; two new resonance lines (397.112 and 423.344 Å) and three transitions to levels of $4p^45p$
2. $(^3P)^4D_{7/2}$ – new level; four strong transitions to levels of $4p^45p$
3. $(^1S)^2D_{5/2}$ – new level; one new resonance line (307.148 Å) and three transitions to levels of $4p^45p$
4. $(^3P)^4F_{7/2}$ – present in [6]; five transitions to levels of $4p^45p$
5. $(^3P)^4F_{9/2}$ – new level; single line at 602.387 Å, places $(^3P)^4F_{9/2}$ close to prediction
6. $(^3P)^2F_{7/2}$ – new level; six transitions to levels of $4p^45p$
7. $(^1D)^2G_{7/2}$ – new level; four transitions to levels of $4p^45p$
8. $(^1D)^2G_{9/2}$ – present in [6]; single line at 600.282 Å; places $(^1D)^2G_{9/2}$ close to prediction
9. $(^1D)^2F_{7/2}$ – present in [6]; six transitions to levels of $4p^45p$

We note that the two $J=9/2$ levels of $4p^44d$ are established by single transitions that are close in wavelength, 600.282 Å and 602.387 Å. Thus, one could consider interchanging their classifications without changing the level values very much. Our present classifications were chosen to provide the best match with the level values given by the least-squares fit (LSF) with the Cowan code, described in Sec. 4 below.

The structure of the $4p^44d$ configuration is shown in figure 2. This is similar to figure 1 of [4], except that we show here the observed positions of levels that were previously unknown.

3.2 $4s^24p^45s$ levels

The $4s^24p^45s$ levels [1,2,4] have improved values due to their combinations with $4s^24p^45p$. For completeness, in figure 3 we give the structure of the $4p^45s$ configuration. This is the same as figure 2 of [4], except that here we designate the levels in jI coupling, rather than JIj . This coupling scheme is more now more commonly used for np^4ns configurations.

3.3 $4s^24p^45p$ levels

As already mentioned, all levels of this configuration were given in [6]. However, we find that 13 of the 21 levels of this configuration given in [6] were spurious. The following levels from [6] have been replaced by new levels in table 2 (We use here the LS designations from [6], although for this coupling scheme, it is not possible to specify the J-value of the core term.):

1. $(^3P_2)^4P_{3/2}$ at 423114; now 5p13 at 421257.96 cm^{-1}
2. $(^3P_2)^4P_{5/2}$ at 424592; now 5p15 at 421991.19 cm^{-1}
3. $(^3P_1)^2P_{1/2}$ at 436172; now 5p21 at 434797.76 cm^{-1}
4. $(^3P_2)^4D_{3/2}$ at 437474; now 5p23 at 435427.69 cm^{-1}
5. $(^3P_0)^4D_{1/2}$ at 438427; now 5p31 at 436859.11 cm^{-1}
6. $(^3P_2)^2P_{3/2}$ at 440224; now 5p33 at 437477.01 cm^{-1}
7. $(^3P_0)^4S_{3/2}$ at 444078; now 5p43 at 442453.66 cm^{-1}
8. $(^3P_1)^2D_{3/2}$ at 445849; now 5p53 at 444879.34 cm^{-1}
9. $(^3P_1)^2S_{1/2}$ at 447709; now 5p41 at 444340.07 cm^{-1}
10. $(^1D_2)^2F_{7/2}$ at 452408; now 5p27 at 452999.87 cm^{-1}
11. $(^1D_2)^2P_{3/2}$ at 472926; now 5p73 at 459077.64 cm^{-1}
12. $(^1S_0)^2P_{3/2}$ at 483178; now 5p83 at 484897.26 cm^{-1}
13. $(^1S_0)^2P_{1/2}$ at 487131; now 5p61 at 482699.28 cm^{-1}

The structure of the $4p^45p$ levels is shown in figure 4. The levels are designated in jI -coupling.

3.4 $4s^24p^45d$ and $4s^24p^46s$ levels

The structures of the $4p^45d$ and $4p^46s$ configurations are shown in figure 5. As these configurations lie very close in energy, we treat them together.

A number of $4p^45d$ and $4p^46s$ levels were established by Chaghtai et al [5], based on their observation of resonance lines in the 174-200 Å region. They reported almost all of the levels that could make transitions to the ground term, that is levels with $J=1/2, 3/2$ or $5/2$. Only $4p^4(^3P)5d\ ^4D_{5/2}$ was missing. These levels were given again in [6], some with improved accuracy. Our present work confirms most of these levels, improves their accuracies, and provides values for the $J=7/2, 9/2$ levels, which cannot radiate to the ground term. Five of the levels of [5,6] were found to be spurious, and several J-values were revised.

The spurious levels were $4p^4(^3P)5d\ ^4P_{1/2}$, $4p^4(^1S)5d\ ^2D_{3/2}$, $4p^46s\ (^3P_2)_{5/2}$, $4p^46s\ (^3P_0)_{1/2}$, and $4p^46s\ (^1S_0)_{1/2}$ (designations from [6]). We confirm the level $4p^46s(^1D_2)_{5/2}$ given in [5] (573105 cm^{-1}), but reject the revised value given in [6] (573135 cm^{-1}). Our present value is 573101.84 cm^{-1} .

Our results for the $4p^45d$ and $4p^46s$ levels are given in table 3. Although this is a complete set, for some levels only tentative values can be given:

1. The $4p^45d\ (^3P_2)[0]_{1/2}$ level (5d21) is established by two lines: $192.182\text{ \AA}$ to $p5\ 3$ and $1055.966\text{ \AA}$ to $5p11$. However, the $192.182\text{-\AA}$ line is largely obscured by a strong line of O IV and so was given a large uncertainty in the level optimization. The value of $4p^45d\ (^3P_2)[0]_{1/2}$ is thus based almost entirely on $1055.966\text{ \AA}$, $5d21\text{-}5p11$. A possible confirming transition predicted at $1008.876\text{ \AA}$, $5d21\text{-}5p13$, was not observed. This could occur because of our use of a filter to eliminate higher order lines that has low-wavelength cutoff near $1000\text{ \AA}$. The level is thus uncertain and was not included in the LSF.
2. The $4p^45d\ (^1D_2)[4]_{7/2}$ level (5d47) is established by a single line, $1081.130\text{ \AA}$, $5d47\text{-}5p45$. This transition is predicted to be extremely strong, so this is likely correct. However, $1081.130\text{ \AA}$ is also classified as $5d17\text{-}5p15$. We thus consider $4p^45d\ (^1D_2)[4]_{7/2}$ to be tentative and exclude it from the LSF.
3. The $4p^45d\ (^1D_2)[3]_{7/2}$ level (5d57) is established by a single line, $1061.816\text{ \AA}$, $5d57\text{-}5p27$. This transition is predicted to be strong, so this is likely correct. A possible confirming transition $5d55\text{-}5d57$ cannot be observed due to the presence of a strong line of Si III. Unfortunately, $1061.816\text{ \AA}$ is also classified as $5d33\text{-}5p21$, which makes our value for $5d57$ tentative at best. It was not included in the LSF.
4. The $4p^45d\ (^3P_2)[4]_{9/2}$ level (5d19) is established by a single line, $1114.688\text{ \AA}$, $5d19\text{-}5p17$. This transition is predicted to be strong, so this is likely correct. However, since there are no confirming transitions, we consider the level to be tentative.
5. The $4p^45d\ (^1D_2)[4]_{9/2}$ level (5d29) is established by a single line, $1115.532\text{ \AA}$, $5d29\text{-}5p27$. This transition is predicted to be strong, so this is likely correct. However, since there are no confirming transitions, we consider the level to be tentative.

As can be seen, the lines that establish $5d19$ and $5d29$, $1114.688\text{ \AA}$ and $1115.532\text{ \AA}$, have nearly the same wavelength. The matching of these two lines with the $5d19$ and $5d29$ levels was done so as to produce the best agreement with the LSF predictions. An effort was made to resolve the question by an isoelectronic comparison. However, the lines were again predicted to be so close that a clear resolution was not possible. In table 3, we list alternative values for the $5d19$ and $5d29$ levels that would apply if the designations were interchanged.

3.5 Higher $4p^4nd$ and $4p^4ns$ levels

In [5] some levels of these configurations were located on the basis of resonance lines in the region around $159\text{ \AA}$. In [6] a number of these levels were reported to make transitions to

levels of $4p^45p$. In our present observations many of these lines do not appear as belonging to Zr VI, and we thus conclude that the results for these configurations in [5,6] cannot be accepted without further confirmation.

4. Theoretical Interpretation

4.1 Odd parity configurations

As in [11] “The observed configurations were interpreted theoretically by making least-squares fits of the energy parameters to the observed levels with the Cowan suite of codes, RCN (Hartree-Fock), RCG (energy matrix diagonalization), and RCE (least-squares parameter fitting) [12]. The Hartree-Fock code was run in a relativistic mode (HFR) with a correlation term in the potential. Breit energies were not included. For the initial calculations the HFR values were scaled by factors of 0.85 for the direct electrostatic parameters F^k , the exchange electrostatic parameters G^k , and the configuration interaction parameters R^k .” The odd configurations $4s^24p^5$, $4s^24p^45p$, $4s^24p^44f$, and $4s4p^54d$ were treated as a single group.

The Hartree-Fock and least-squares fitted parameters for the odd configurations are given in table 4. For these calculations, the $4p^45p$ exchange electrostatic parameters, $G^0(4p5p)$ and $G^2(4p5p)$, were linked at their HFR ratio. The LSF/HFR ratio of 0.856 is satisfactory. The configuration interaction (CI) parameters for the $4s^24p^5$ - $4s^24p^45p$ interaction were held fixed at their scaled HFR values. All other CI parameters and parameters for $4s^24p^44f$ and $4s4p^54d$ were fixed at their scaled HFR values. The value of the effective interaction parameter $\alpha(4p4p)$ for the $4p^45p$ configuration was fixed at the value observed for the $4p^4$ core of Zr VII [15]. In table 4 only values for the observed configurations $4s^24p^5$ and $4s^24p^45p$ are given.

The calculated level values and eigenvector compositions for the odd configurations are given in table 5. This table gives the percentage compositions for the three leading eigenvector states in LS-coupling and the percentage for the leading eigenvector state in $j\bar{j}$ -coupling. As can be seen there is not much mixing between the $4s^24p^5$ and the $4s^24p^45p$ configurations. Their mutual repulsion is only about 320 cm^{-1} .

4.2 Even parity configurations

The parameters for the even configurations are given in table 6. Here, the $4s4p^6$, $4p^44d$, $5s$, $5d$, $6s$, $6d$, and $7s$ configurations were treated as single group. For the initial calculations the HFR values were scaled by factors of 0.85 for the direct electrostatic parameters F^k , the exchange electrostatic parameters G^k , and the configuration interaction parameters R^k . All the parameters that were allowed to vary were well defined in the fit and have reasonable ratios to the HFR values. The exchange parameters $G^1(4p5d)$ and $G^3(4p5d)$ were linked at their HFR ratio. The CI parameters for the $4s4p^6$ - $4s^24p^44d$ and $4s4p^6$ - $4s^24p^45d$ interactions were also linked at their HFR ratio. The fitted values are reasonable. The other CI parameters and those for $4p^46d$ and $4p^47s$ were held fixed at their scaled HFR values. As described in [4] the interaction of $4s4p^6\ ^2S_{1/2}$ with the $4s^24p^4(^1D)4d\ ^2S$ level is great, with a mutual repulsion of $\sim 33000\text{ cm}^{-1}$. On the other hand, interaction between $4s4p^6$ and $4s^24p^45d$ is negligible. The value of the effective interaction parameter $\alpha(4p4p)$ for the

$4p^44d$, $5s$, $5d$, and $6s$ configurations was again fixed at the value observed for the $4p^4$ core of Zr VII [15]. The calculated level values and eigenvector compositions for the even levels are given in table 7. This table gives the percentage compositions for the three leading eigenvector states in LS-coupling and the percentage for the leading eigenvector state in jl -coupling, where appropriate. As can be seen, the purity of the states of the $4p^44d$ configuration in LS-coupling is low, leading to low leading percentages for many of the levels. In order to avoid duplicate names, we have used the second component for the level observed at 279457 cm^{-1} to designate the level. Even though the $4p^45d$ and $4p^46s$ configurations are practically coincident, there is not much mixing of states. The percentage compositions for the $4s4p^6$, $4s^24p^44d$, and $4s^24p^45s$ configurations are close to those given in [4].

5. $4s4p^6$ - $4s^24p^45p$ transitions

Transitions between the $4s4p^6$ and $4s^24p^45p$ configurations are normally forbidden as two electron jumps. However, because of configuration interaction between $4s4p^6$ and $4s^24p^44d$, they can in fact take place. We observe six of them in Zr VI. In lower members of the isoelectronic sequence, these transitions occur at wavelengths that are long relative to the resonance lines and serve to improve the accuracy of the excited levels. However, as the separation of configurations with different principal quantum number increases with increasing ionization stage, these transitions move to lower wavelength, and their inclusion does not improve the accuracy of the excited levels. For Zr VI, these transitions fall in the same wavelength region as the $4s^24p^5$ - $4s^24p^44d$ resonance transitions, so they have practically no effect on the Ritz values for the resonance lines.

6. Ritz wavelengths

We determined Ritz wavelengths for a number of the lines by differencing the energy level values in tables 2 and 3. The uncertainties of the calculated wavelengths were taken to correspond to the square root of the sum of the squares of the uncertainties of the combining levels. In table 1 we show the Ritz wavelengths and uncertainties for lines likely to be suitable as wavelength standards, that is where the uncertainty of the Ritz wavelength is $\pm 0.0020\text{ \AA}$ or less. (This table contains all observed lines together with those with Ritz values.) The Ritz values have uncertainties that vary from $\pm 0.0003\text{ \AA}$ to $\pm 0.0020\text{ \AA}$.

7. Oscillator strengths

Table 1 lists the transition probabilities $g_U A$ and $\log g_L f$ for each observed line as calculated with wave functions obtained from the fitted energy parameters. Here, f is the oscillator strength, g_U is the statistical weight of the upper level $2J_U+1$ and g_L is the statistical weight of the lower level $2J_L+1$. The A-values are compared with recently published *ab initio* values in section 9 below.

Since there are no experimental values for the transition probabilities of Zr VI, it is difficult to estimate the uncertainty of the calculated values. One guide is the cancellation factor. This is the ratio of the calculated transition probability to a value calculated with all parts of the

wave function taken as positive [12]. Low cancellation factors generally indicate a larger uncertainty in the calculated values. Indeed, many of the values in table 1 have low cancellation factors. To try to obtain a more quantitative estimate of the uncertainties, we attempted to judge the sensitivity of the values to the parameter values used for the calculation. For this, an alternate calculation was performed with parameters that varied by small amounts from those used for the main calculation. The differences in the results were then used to put the uncertainties on a semi-quantitative basis with code letters, as are often used for this purpose. The letter codes define categories of uncertainties in A -values: C (25 %), D+ (40 %), D (50 %), E (>50 %).

8. Ionization energy

In [4] an estimated value of $n^*(4p^45s)$ of 3.12 ± 0.02 was used to determine an ionization energy of $773000 \pm 5000 \text{ cm}^{-1}$. In [6] this was revised upward to $776500 \pm 500 \text{ cm}^{-1}$ on the basis of a Ritz diagram for the $4p^45s$, $6s$, and $7s$ configurations. (No details of the determination were given.) Since four of the eight levels of $4p^46s$ in [6] have now been found to be spurious, this value must be re-determined.

For our new determination we use the centers-of-gravity of the $4p^45s$ and $4p^46s$ configurations together with an estimated value for the change in effective quantum number $n^*(4p^46s-4p^45s) = n^*(4p^46s) - n^*(4p^45s)$. This allows us to find the limit of the $4p^4\infty s$ series, which is the center-of-gravity of the $4p^4$ configuration of Zr VII.

From the observed levels in table 3, we find the centers-of-gravity of the $4p^45s$ and $4p^46s$ configurations as 383198.13 and 562514.9 cm^{-1} , respectively. Our value for $n^*(4p^46s-4p^45s)$ is taken from $n^*(4p^66s-4p^65s)$ for the one-electron atom Mo VI [16], 1.0338. We use Cowan's Hartree-Fock code to estimate the change in going from Mo VI to Zr VI. For Mo we calculate $n^*(4p^66s-4p^65s)$ as 1.0367 and for Zr VI we calculate $n^*(4p^46s-4p^45s)$ as 1.0341, a difference of 0.0026. We thus estimate $n^*(4p^46s-4p^45s)$ for Zr VI as $1.0338 - 0.0026 = 1.0312$, with an estimated uncertainty of ± 0.0015 . This produces a limit of $793780 \pm 300 \text{ cm}^{-1}$. The effective quantum numbers for Zr VI are $n^*(5s) = 3.102(1)$ and $n^*(6s) = 4.133(3)$. Correcting for the energy of the center-of-gravity of $4p^4$ in Zr VII, 16402 cm^{-1} [15], we obtain for the ionization energy of Zr VI the value $777380 \pm 300 \text{ cm}^{-1}$ ($96.38 \pm 0.04 \text{ eV}$) [17].

9. Comparison with *ab initio* calculations

Recently, two sets of *ab initio* calculations for the levels and oscillator strengths of Zr VI have appeared. Singh et al [18] used a multiconfiguration Dirac-Fock approach to make calculations for transitions within the $n=4$ complex; $4s^24p^5$, $4s4p^6$, $4s^24p^4d$. Aggarwal and Keenan [19] used the general-purpose relativistic atomic structure package GRASP for calculations within the same complex of $n=4$ configurations. Both calculations are based on new versions of the Grant atomic structure code, as described in their papers [18,19]. Froese Fischer [20] has recently discussed the accuracy that might be expected from calculations for complex atoms with GRASP, in particular as applied to the Br-like ion W^{39+} . Aggarwal and Keenan also used the Flexible Atomic Code [21].

A comparison of the results of the *ab initio* calculations [18, 19] for the wavelengths and transition probabilities with our present values is given in table 8. The wavelengths for Aggarwal and Keenan [19] in this table are differences of the GRASP3 energies in their table 4. Overall, the wavelengths obtained by Singh et al [18] are in better agreement with our present observed wavelengths than those of Aggarwal et al [19]. A notable disagreement for the transition probabilities is for the $4s^2 4p^5 \ ^2P_{3/2} - 4s^2 4p^4 d \ (^3P)^4F_{3/2}$ transition (indices 1-12), observed at 368,600 Å. (The indices are sequential numbers used in [18] and [19] in their enumeration of the energy levels.) Both Singh et al [18] and Aggarwal and Keenan [19] find an extremely low transition probability. However, we obtain a fairly high A-value, and it is indeed observed as a fairly strong line. This transition is nominally forbidden as an inter-combination line in LS-coupling because of the change of spin. However, although the $4p^4 d$ level (271296 cm⁻¹ observed value) has a leading percentage composition in LS coupling of 47% $4p^4 d \ (^3P)^4F_{3/2}$, the full percentage compositions show that it actually has a total doublet character of about 36%. This accounts for our calculated transition probability and observed line strength. Singh et al [18] report a composition of 74% $4p^4 d \ (^3P)^4F_{3/2}$ for this level, with no secondary percentage mentioned. Percentage compositions were not reported by Aggarwal and Keenan [19].

A number of other striking differences can be seen in table 8. The values found by all three calculations for the $4s^2 4p^5 \ ^2P_{3/2} - 4s^2 4p^4 d \ (^1S)^4D_{5/2}$ transition (indices 1-26) are extremely discrepant. The present value is about in the middle of the two found with GRASP. The values for the $4s^2 4p^5 \ ^2P_{1/2} - 4s^2 4p^4 d \ (^3P)^4D_{3/2}$ transition (indices 2-6) also disagree by a large amount. Still, they all predict that this will be a very weak line, and in fact it has not been observed.

Both Singh et al [18] and Aggarwal and Keenan [19] compare their calculated level values with the observed values given in the NIST Atomic Spectra Database [22]. Since we have made a number of revisions to the $4p^4 d$ levels, a new comparison is called for. This is given in table 9.

The percentage compositions for the states of the $4s4p^6$ and $4s^2 4p^4 d$ configurations obtained in the present work are compared with those obtained in the MCDF calculations of Singh et al. [18] in table 10. The general agreement is qualitatively reasonable. However, there are some striking differences. For example, as a result of the large $4s4p^6 \ ^2S_{1/2} - 4s^2 4p^4 d \ (^1D)^2S_{1/2}$ interaction mentioned above, we find that the level designated as $4s4p^6 \ ^2S_{1/2}$ (index 3) has an admixture of 23% $4p^4 d \ (^1D)^2S_{1/2}$. Singh et al. [18] find a similar admixture for this level. Correspondingly, we find the level designated as $4p^4 d \ (^1D)^2S_{1/2}$ (index 28) to have an admixture of 20% $4s4p^6 \ ^2S_{1/2}$, as would be generally expected. No such admixture is given by Singh et al. [18]. Presumably, their $4s4p^6 \ ^2S_{1/2}$ percentage calculated for this state is below about 16%, the lowest percentage present in their table 3. Other striking differences can be seen for the levels at 271296 (index 12), 272834 (index 14), 279457 (index 18), and 346346 (index 29) cm⁻¹. Of course, the calculated oscillator strengths depend largely on the admixtures represented by the percentages.

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Figure 1.

Schematic overview of the configurations of Zr VI. The calculated positions of the 4s²4p⁴f and 4s4p⁶4d configurations, for which no levels are known, are also shown.

Figure 2.
Structure of the $4s^2 4p^4 4d$ configurations of Zr VI.

Figure 3. Structure of the $4s^2 4p^4 5s$ configurations of Zr VI. The levels are designated in j -coupling.

Figure 4. Structure of the $4s^2 4p^4 5p$ configuration of Zr VI . The levels are designated in j/l -coupling.

Figure 5.

Structures of the $4s^24p^45d$ and $4s^24p^46s$ configurations of Zr VI. The levels are designated in jI -coupling. The $4s^24p^46s$ levels are shown as dashed. Levels noted by open circles are tentative.

Table 1

Observed spectral lines of Zr VI. Wavelengths and wave numbers are in vacuum. Wavelength values in parentheses are Ritz values. General uncertainty of the observed wavelengths is ± 0.005 Å. Uncertainties for less certain wavelengths are given in section 2 of text. Acc. is the accuracy estimate.

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	Unc($\Delta\lambda_{\text{Ritz}}$, Å)	$g_u/A(\text{s}^{-1})$	$\log(gf)$	CF	Acc.
165.930	5	602664	6s31	p5 3	165.9308	0.0011	2.28E+09	-2.03	0.15	D+
170.342	6	587054	6s31	p5 1	170.3408	0.0012	6.37E+09	-1.56	0.60	D+
174.066	6	574495	5d85	p5 3	174.0660	0.0003	2.46E+09	1.95	0.30	D+
174.489	70	573102	6s25	p5 3	174.4891	0.0003	2.27E+10	0.99	0.65	D+
178.236	50	561054	6s21	p5 3	178.2371	0.0003	9.00E+09	1.37	0.54	D+
178.776	60	559359	6s23	p5 3	178.7769	0.0003	8.48E+09	1.39	0.55	D+
178.794	30	559303	5d83	p5 1	178.7993	0.0004	6.19E+09	1.53	0.26	D+
179.144	10	558210	6s11	p5 3	179.1445	0.0003	1.17E+09	2.25	0.51	E
179.308	70	557700	6s33	p5 1	179.3084	0.0003	2.14E+10	0.99	0.70	D+
182.213	30	548808	5d73	p5 3	182.2139	0.0003	3.07E+09	1.82	0.16	D+
182.550	20	547795	5d51	p5 3			4.24E+09	1.67	0.14	D+
182.657	90	547474	6s13	p5 3	182.6578	0.0003	1.86E+10	1.03	0.25	D+
182.744	80	547214	5d75	p5 3	182.7439	0.0003	1.34E+10	1.18	0.45	D+
183.262	70	545667	5d65	p5 3	183.2623	0.0003	9.69E+09	1.31	0.35	D+
183.336	60	545447	6s15	p5 3	183.3357	0.0004	2.33E+09	1.93	0.67	D+
183.336	60	545447	6s21	p5 1	183.3471	0.0003	1.07E+10	1.27	0.40	D+
183.680	90	544425	5d63	p5 3			3.65E+10	0.73	0.50	D+
183.908	5	543750	6s23	p5 1	183.9068	0.0004	1.19E+09	2.22	0.35	E
184.063	60	543292	5d41	p5 3	184.0618	0.0003	6.50E+09	1.48	0.17	D+
187.075	20	534545	5d53	p5 3	187.0723	0.0003	2.64E+09	1.86	0.06	D+
187.361	100	533729	5d55	p5 3	187.3582	0.0003	2.74E+10	0.84	0.41	D+
187.549	80	533194	5d73	p5 1	187.5459	0.0004	2.50E+10	0.88	0.42	D+
187.830	5	532396	5d45	p5 3	187.8277	0.0003	1.04E+09	2.26	0.25	E
187.905	60	532184	5d51	p5 1			1.67E+10	1.05	0.44	D+
188.490	20	530532	5d43	p5 3	188.4876	0.0003	2.23E+09	1.93	0.20	D+
188.912	2	529347	5d35	p5 3	188.9103	0.0003	1.89E+08	3.00	0.05	E
189.046	3	528972	5d33	p5 3	189.0444	0.0003	7.85E+08	2.38	0.31	E

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_U f)$	CF	Acc.
189.101	30	528818	5d63	p5 1			6.39E+09	1.47	0.29	D+
189.267	2	528354	5d31	p5 3	189.2658	0.0003	3.84E+08	2.69	0.11	E
189.506	5	527688	5d41	p5 1	189.5041	0.0004	4.92E+08	2.58	0.02	E
191.557	90	522038	5d25	p5 3	191.5577	0.0003	2.73E+10	0.82	0.43	D+
191.666	80	521741	5d23	p5 3	191.6663	0.0004	1.43E+10	1.10	0.42	D+
192.182	20	520340	5d21	p5 3	192.1679	0.0004	2.51E+09	1.86	0.20	D+
192.696	60	518952	5d53	p5 1	192.6968	0.0004	7.84E+09	1.36	0.23	D+
194.108	1	515177	5d13	p5 3	194.1104	0.0003	5.39E+07	3.52	0.01	E
194.197	20	514941	5d43	p5 1	194.1988	0.0004	2.32E+09	1.88	0.12	D+
195.024	2	512757	5d31	p5 1	195.0250	0.0004	4.35E+08	2.61	0.08	E
197.575	80	506137	5d23	p5 1	197.5749	0.0005	1.90E+09	1.95	0.05	D+
236.281	100	423225	5s31	p5 3	236.2818	0.0005	3.14E+09	1.58	0.06	D+
245.327	90	407619	5s31	p5 1	245.3261	0.0006	1.62E+10	0.84	0.47	D+
253.678	80	394201	5s33	p5 3	253.6812	0.0005	2.26E+09	1.66	0.04	D+
254.092	400	393558	5s25	p5 3	254.0939	0.0005	6.20E+10	0.22	0.65	C
259.888	200	384781	5s21	p5 3	259.8878	0.0006	2.91E+10	0.53	0.67	D+
263.310	500	379780	5s23	p5 3	263.3127	0.0006	4.96E+10	0.29	0.83	C
264.142	90	378584	5s33	p5 1	264.1361	0.0007	4.67E+10	0.31	0.61	C
264.940	100	377444	5s11	p5 3	264.9343	0.0006	6.57E+08	2.16	0.15	D+
270.480	200	369713	5s13	p5 3	270.4811	0.0006	6.60E+10	0.14	0.74	C
270.872	200	369178	5s21	p5 1	270.8716	0.0007	3.75E+10	0.39	0.61	C
274.105	200	364824	5s15	p5 3	274.1024	0.0006	2.76E+09	1.51	0.33	D+
274.598	100	364169	5s23	p5 1	274.5941	0.0007	4.14E+09	1.33	0.24	D+
276.364	80	361842	5s11	p5 1	276.3582	0.0007	2.53E+07	3.54	0.01	E
279.198	90	358169	4d83	p5 3	279.1985	0.0007	1.78E+10	0.68	0.05	D+
282.400	90	354108	5s13	p5 1	282.3990	0.0008	3.56E+09	1.37	0.10	D+
288.730	200	346344	4d51	p5 3	288.7290	0.0008	2.75E+10	0.46	0.11	D+
290.949	500	343703	4d85	p5 3	290.9433	0.0007	1.05E+12	1.12	0.85	C
291.920	500	342560	4d83	p5 1	291.9151	0.0009	6.60E+11	0.93	0.85	C
294.395	500	339680	4d73	p5 3	294.3923	0.0007	5.84E+11	0.88	0.90	C
298.779	300	334696	4d41	p5 3	298.7796	0.0008	2.81E+11	0.58	0.71	C

$\lambda_{obs}(\text{\AA})$	Intensity	$\sigma_{obs}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{Ritz}(\text{\AA})$	$Unc(\lambda_{Ritz}, \text{\AA})$	$g_U(A(s^{-1}))$	$\log(g_U f)$	CF	Acc.
302.351	300	330741.4	4d51	p5 1	302.3498	0.0010	2.56E+11	0.55	0.87	C
307.148	30	325575.9	4d75	p5 3	307.1472	0.0010	3.16E+06	4.35	0.00	E
308.569	100	324076.6	4d73	p5 1	308.5658	0.0009	4.65E+09	1.18	0.02	D+
313.150	300	319335.8	4d63	p5 3	313.1496	0.0010	1.27E+10	0.73	0.11	D+
313.389	300	319092.2	4d41	p5 1	313.3891	0.0010	2.55E+10	0.43	0.11	C
329.242	300	303728.0	4d63	p5 1	329.2361	0.0012	1.31E+10	0.67	0.06	D+
333.768	400	299609.3	4d65	p5 3	333.7687	0.0010	2.97E+09	1.31	0.10	D+
340.915	30	293328.2	4p61	5p83	340.9169	0.0011	1.38E+09	1.62	0.02	E
343.493	10	291126.7	4p61	5p61	343.4908	0.0011	2.34E+07	3.38	0.02	E
348.262	200	287140.1	4d55	p5 3	348.2592	0.0012	9.38E+08	1.77	0.01	D+
353.221	250	283108.9	4d45	p5 3	353.2171	0.0011	2.40E+09	1.35	0.01	D+
357.837	30	279456.8	4d53	p5 3	357.8365	0.0012	2.21E+08	2.37	0.00	D+
358.755	300	278741.8	4d35	p5 3	358.7544	0.0012	1.71E+09	1.48	0.02	D+
364.080	300	274664.9	4d43	p5 3	364.0791	0.0013	1.52E+09	1.52	0.01	D+
366.095	60	273153.1	4p61	5p51	366.0947	0.0012	9.72E+08	1.71	0.18	D+
366.522	200	272834.9	4d33	p5 3	366.5226	0.0014	2.11E+09	1.37	0.02	D+
367.523	300	272091.8	4d31	p5 3	367.5238	0.0015	1.72E+09	1.46	0.15	D+
368.494	300	271374.8	4d25	p5 3	368.4947	0.0015	1.28E+09	1.58	0.61	D+
368.600	250	271296.8	4d23	p5 3	368.6010	0.0013	8.52E+08	1.76	0.01	D+
375.546	30	266279.0	4d21	p5 3	375.5467	0.0015	2.99E+07	3.20	0.00	E
378.342	60	264311.1	4p61	5p63	378.3472	0.0013	1.61E+09	1.46	0.27	D+
378.992	80	263857.8	4d53	p5 1	378.9969	0.0015	6.03E+07	2.89	0.00	E
386.007	250	259062.7	4d43	p5 1	386.0068	0.0016	1.55E+09	1.46	0.01	D+
388.754	20	257232.1	4d33	p5 1	388.7546	0.0018	3.39E+07	3.12	0.00	E
389.881	100	256488.5	4d31	p5 1	389.8811	0.0019	1.43E+08	2.49	0.01	E
391.094	100	255693.0	4d23	p5 1	391.0936	0.0017	3.67E+07	3.07	0.00	E
397.112	30	251818.1	4d11	p5 3			2.79E+07	3.18	0.01	E
398.588	2	250885.6	4p61	5p43	398.5922	0.0014	2.20E+08	2.28	0.15	D+
398.919	80	250677.5	4d21	p5 1	398.9218	0.0019	1.53E+08	2.44	0.00	E
399.967	80	250020.6	4d13	p5 3	399.9718	0.0018	4.90E+07	2.93	0.00	E
401.701	80	248941.4	4d15	p5 3	401.7031	0.0019	5.69E+07	2.86	0.00	E

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_U f)$	CF	Acc.
411.136	4	243228.5	4p61	5p21	411.1384	0.0016	7.96E+07	2.70	0.08	E
423.344	5	236214.5	4d11	p5 1			1.93E+07	3.29	0.00	E
514.611	1	x 194321.5	4d13	5p41			2.32E+08	2.04	0.07	D+
516.763	10	193512.3	4d15	5p43			7.64E+08	1.52	0.06	D+
516.970	10	x 193434.8	4d27	5p55	516.9686	0.0014	3.09E+08	1.91	0.06	E
522.000	2000	191570.9	4p61	p5 3			2.62E+09	0.97	0.04	D+
522.929	20	191230.5	4d17	5p35			1.95E+09	1.10	0.08	D+
524.835	5	190536.1	4d13	5p35			2.97E+08	1.91	0.06	D+
530.404	5	x 188535.5	4d15	5p33			1.43E+08	2.22	0.01	D+
532.528	10	s 187783.6	4d23	5p73	532.5335	0.0017	6.94E+08	1.53	0.11	D+
533.450	30	187459.0	4d13	5p33			7.08E+08	1.52	0.10	D+
535.216	80	186840.5	4d13	5p31			1.16E+09	1.30	0.12	D+
538.618	5	185660.3	4d11	5p33			3.24E+08	1.85	0.12	D+
539.350	70	1,x 185408.4	4d13	5p23			3.38E+07	2.83	0.00	E
539.765	10	1,x 185265.8	4d53	5p51	539.7620	0.0014	1.46E+08	2.20	0.02	D+
540.791	40	184914.3	4d43	5p55	540.7885	0.0015	1.06E+09	1.33	0.24	E
541.756	10	x 184584.9	4d23	5p63	541.7643	0.0017	1.56E+08	2.16	0.02	D+
542.264	60	184412.0	4d43	5p73	542.2639	0.0015	1.15E+09	1.30	0.08	D+
544.117	10	183784.0	4d31	5p63			2.25E+08	2.00	0.09	D+
546.182	80	183089.2	4d37	5p55			1.27E+09	1.24	0.10	D+
546.508	50	p,x 182979.9	4d11	5p21			1.59E+09	1.15	0.19	D+
556.729	80	179620.6	4d53	5p73	556.7295	0.0013	5.98E+08	1.55	0.07	D+
559.569	200	178709.0	4d15	5p17			1.54E+09	1.14	0.55	D+
560.428	2	x 178435.1	4d23	5p45	560.4292	0.0018	2.26E+08	1.97	0.14	D+
560.769	300	178326.5	4d17	5p17			9.64E+09	0.34	0.71	C
561.601	10	x 178062.4	4d21	5p41			1.88E+08	2.05	0.03	D+
562.444	300	177795.5	4d17	5p25			4.34E+09	0.69	0.33	C
564.537	200	177136.3	4d35	5p63	564.5382	0.0015	1.19E+09	1.25	0.16	D+
565.300	5	x 176897.2	4d33	5p45			6.70E+07	2.49	0.10	D+
566.546	20	1 176508.2	4d37	5p27			1.65E+08	2.10	0.03	D+
566.670	300	p 176469.6	4d45	5p55	566.6725	0.0013	5.13E+09	0.61	0.34	C

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_L f)$	CF	Acc.
566.819	300	176423.2	4d53	5p63	566.8261	0.0014	2.37E+09	0.94	0.18	D+
567.620	80	176174.2	4d21	5p43			4.59E+08	1.65	0.14	D+
568.284	2000	175968.4	4p61	p5 1			1.19E+09	1.24	0.05	D+
569.281	300	175660.2	4d13	5p11			2.08E+09	1.00	0.27	D+
573.360	300	174410.5	4d27	5p35			5.60E+09	0.56	0.17	C
575.179	500	173858.9	4d11	5p11			3.29E+09	0.79	0.58	D+
576.090	10	173584.0	4d23	5p53	576.0923	0.0019	5.03E+07	2.60	0.01	E
577.233	20	173240.3	4d37	5p45			2.04E+09	0.99	0.09	D+
577.863	500	173051.4	4d15	5p15			1.10E+10	0.26	0.69	C
578.737	100	172790.1	4d31	5p53			9.14E+08	1.34	0.18	D+
578.811	80	172768.0	4d45	5p63	578.8171	0.0014	8.03E+08	1.40	0.05	D+
579.142	400	172669.2	4d17	5p15			1.47E+10	0.13	0.43	C
579.913	200	172439.7	4d55	5p55	579.9174	0.0018	1.38E+09	1.15	0.22	D+
580.321	300	172318.4	4d15	5p13			7.13E+09	0.45	0.36	C
581.236	200	172047.2	4d33	5p53			1.44E+09	1.14	0.26	D+
581.480	300	171975.0	4d13	5p15			2.49E+09	0.90	0.66	D+
581.610	200	171936.5	4d55	5p73	581.6144	0.0018	1.34E+09	1.16	0.18	D+
583.063	200	171508.1	4d33	5p41			1.59E+09	1.09	0.33	D+
583.970	400	171241.7	4d13	5p13			7.86E+09	0.40	0.68	C
584.111	150	171200.3	4d21	5p33			9.04E+08	1.33	0.34	D+
584.251	250	171159.3	4d23	5p43	584.2568	0.0020	1.67E+09	1.07	0.25	D+
584.517	200	171081.4	4d25	5p43			9.33E+08	1.32	0.27	D+
586.229	100	170581.8	4d21	5p31			8.86E+08	1.34	0.26	D+
588.625	200	169887.4	4d45	5p27	588.6235	0.0015	1.42E+09	1.13	0.36	D+
589.367	5	169673.6	4d43	5p41	589.3639	0.0019	1.98E+08	1.99	0.03	D+
(590.182)		(169439.3)	4d11	5p13			2.20E+09	0.94	0.71	D+
591.079	100	169182.1	4d25	5p35			2.29E+09	0.92	0.35	D+
593.405	200	168519.0	4d21	5p21			3.21E+09	0.77	0.66	D+
595.987	5	167788.9	4d43	5p43	595.9900	0.0019	4.71E+08	1.60	0.07	D+
596.236	5	167718.8	4d33	5p35			3.91E+08	1.68	0.12	D+
598.686	400	167032.5	4d47	5p27			3.31E+09	0.75	0.65	D+

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_L f)$	CF	Acc.
600.282	1000	166588.4	4d29	5p27			3.30E+10	0.25	0.73	C
601.759	2	166179.5	4d23	5p33			1.23E+09	1.18	0.15	D+
601.914	50	166136.7	4d35	5p53	601.9125	0.0017	3.33E+09	0.74	0.21	C
602.040	100	166101.9	4d25	5p33			7.35E+09	0.40	0.59	C
602.387	2000	166006.2	4d19	5p17			3.36E+10	0.26	0.80	C
602.932	5	165856.2	4d55	5p27			5.55E+08	1.52	0.46	D+
604.002	100	165562.4	4d23	5p31			4.62E+09	0.60	0.44	C
604.515	50	165421.9	4d53	5p53	604.5140	0.0016	1.93E+09	0.97	0.29	D+
606.493	50	164882.4	4d53	5p41	606.4912	0.0016	4.18E+09	0.64	0.71	C
607.378	100	164642.1	4d33	5p33			2.27E+09	0.90	0.28	D+
609.525	100	164062.2	4d37	5p35			1.82E+10	0.01	0.78	C
609.552	90	164054.9	4d25	5p23			7.55E+09	0.38	0.76	C
610.639	500	163762.9	4d47	5p45			2.09E+10	0.07	0.65	C
610.834	1000	163710.6	4d35	5p43	610.8309	0.0018	6.00E+09	0.48	0.36	C
611.614	10	163501.8	4d23	5p21			2.05E+09	0.94	0.22	D+
612.145	200	163360.0	4d63	5p61			5.37E+09	0.52	0.48	C
612.234	50	163336.2	4d31	5p23			1.49E+09	1.07	0.40	D+
614.207	5	162811.6	4d43	5p33	614.2076	0.0020	1.51E+09	1.07	0.18	D+
615.047	200	162589.2	4d55	5p45	615.0504	0.0020	2.12E+09	0.92	0.40	D+
616.547	100	162193.6	4d43	5p31	616.5475	0.0020	2.95E+09	0.77	0.41	D+
617.422	200	161963.8	4d33	5p21			2.16E+09	0.91	0.29	D+
617.999	5	161812.6	4d35	5p35	617.9987	0.0019	2.77E+08	1.80	0.06	D+
618.172	200	161767.3	4d45	5p53	618.1718	0.0016	2.80E+09	0.80	0.25	D+
619.181	50	161503.7	4d27	5p17			1.22E+09	1.15	0.23	D+
620.741	2	161097.8	4d53	5p35	620.7415	0.0017	1.53E+08	2.05	0.05	D+
621.223	800	160972.8	4d27	5p25			1.55E+10	0.05	0.80	C
622.037	100	160762.1	4d43	5p23	622.0372	0.0020	3.26E+09	0.72	0.42	C
627.081	200	159469.0	4d65	5p73	627.0812	0.0019	6.98E+09	0.38	0.57	C
627.358	10	159398.6	4d21	5p11			4.46E+08	1.58	0.09	D+
627.583	50	159341.5	4d45	5p43	627.5823	0.0017	2.84E+09	0.78	0.18	D+
627.667	100	159320.1	4d75	5p83			1.54E+10	0.04	0.68	C

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629.982	20	158734.7	4d35	5p33	629.9817	0.0019	1.61E+09	1.02	0.33	D+
632.835	5	158019.1	4d53	5p33	632.8321	0.0017	8.15E+08	1.31	0.11	D+
633.968	200	157736.7	4d55	5p53			7.53E+09	0.34	0.68	C
635.151	50	157442.9	4d45	5p35	635.1510	0.0017	1.27E+09	1.12	0.24	D+
635.318	5	157401.5	4d53	5p31	635.3164	0.0018	4.21E+08	1.59	0.10	D+
638.222	5	156685.3	4d35	5p23	638.2213	0.0020	1.29E+09	1.10	0.14	D+
639.920	200	156269.5	4d65	5p63	639.9202	0.0019	4.09E+09	0.60	0.63	C
640.764	500	156063.7	4d57	5p55			1.65E+10	0.01	0.85	D
641.147	5	155970.5	4d53	5p23	641.1470	0.0018	4.45E+08	1.56	0.07	D+
641.661	500	155845.5	4d27	5p15			3.05E+09	0.73	0.26	C
642.080	40	155743.8	4d25	5p25			8.32E+08	1.29	0.48	D+
643.746	50	155340.8	4d53	5p21	643.7469	0.0019	1.13E+09	1.15	0.20	D+
643.869	400	155311.1	4d55	5p43			4.62E+09	0.54	0.50	C
645.249	2	154978.9	4d21	5p13			3.77E+08	1.62	0.17	D+
646.881	2	154587.9	4d47	5p35			6.90E+08	1.37	0.13	D+
647.745	100	154381.7	4d23	5p11			1.52E+09	1.02	0.38	D+
647.816	100	154364.8	4d45	5p33	647.8152	0.0017	2.33E+09	0.84	0.26	D+
651.100	30	153586.2	4d31	5p11			9.61E+08	1.22	0.78	D+
654.264	2	152843.5	4d33	5p11			1.02E+09	1.19	0.31	D+
655.940	10	152453.0	4d43	5p25			2.88E+08	1.73	0.17	D+
656.533	20	152315.3	4d45	5p23	656.5312	0.0018	1.52E+09	1.01	0.15	D+
661.560	4	151157.9	4d37	5p17			2.67E+08	1.75	0.08	D+
662.196	100	151012.7	4d43	5p11			9.46E+08	1.21	0.15	D+
663.593	5	150694.8	4d23	5p15			3.43E+08	1.65	0.23	D+
663.892	100	150626.9	4d37	5p25			3.94E+09	0.58	0.18	C
663.935	5	150617.2	4d25	5p15			3.00E+08	1.70	0.12	D+
665.185	1	150334.1	4d55	5p33			2.80E+07	2.73	0.01	E
666.124	100	150122.2	4d65	5p45			3.19E+09	0.67	0.40	C
666.835	50	149962.1	4d23	5p13			3.73E+08	1.61	0.10	D+
667.185	10	149883.5	4d25	5p13			2.76E+08	1.74	0.10	D+
668.970	500	149483.5	4d57	5p27			4.62E+09	0.51	0.55	C

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_L f)$	CF	Acc.
670.392	700	149166.5	4d31	5p13			2.13E+09	0.84	0.47	D+
673.754	50	148422.1	4d33	5p13			5.75E+08	1.41	0.11	D+
673.961	100	148376.5	4d35	5p25			1.96E+09	0.88	0.52	D+
674.378	5	148284.8	4d55	5p23			5.80E+08	1.40	0.08	D+
683.926	3	146214.6	4d57	5p45			4.04E+08	1.55	0.07	D+
687.812	50	145388.6	4d63	5p51			2.24E+09	0.80	0.63	C
688.367	5	145271.3	4d65	5p53			7.18E+08	1.29	0.24	D+
694.411	2	144006.9	4d45	5p25			1.44E+08	1.99	0.03	D+
698.082	100	143249.6	4d35	5p15			1.45E+09	0.98	0.27	D+
700.055	5	142845.9	4d65	5p43			4.85E+08	1.45	0.18	D+
701.587	10	142534.0	4d53	5p15			3.91E+08	1.54	0.17	D+
701.674	20	142516.3	4d35	5p13			8.50E+08	1.20	0.11	D+
705.214	2	141800.9	4d53	5p13			9.27E+07	2.16	0.02	D+
708.275	2	141188.1	4d85	5p83	708.2769	0.0020	6.05E+08	1.34	0.10	D+
708.456	5	141152.0	4d47	5p25			5.80E+08	1.36	0.05	D+
709.488	2	140946.7	4d65	5p35			2.36E+08	1.75	0.30	D+
715.604	10	139742.1	4d63	5p73			9.63E+08	1.13	0.27	D+
720.052	10	138878.9	4d45	5p15			4.34E+08	1.47	0.09	D+
723.873	2	138145.8	4d45	5p13			1.22E+08	2.02	0.02	D+
729.724	10	137038.1	4d57	5p35			5.03E+08	1.39	0.15	D+
732.372	5	136542.6	4d63	5p63			7.52E+08	1.22	0.23	D+
736.276	10	135818.6	4d65	5p23			7.16E+08	1.23	0.23	D+
746.246	20	134004.1	4d75	5p55			1.24E+09	0.98	0.55	D+
784.259	50	127508.9	4d65	5p25			3.45E+08	1.50	0.21	D+
789.090	50	126728.3	4d83	5p83			6.11E+08	1.24	0.38	D+
792.305	1	126214.0	6s13	5p13			1.55E+09	0.84	0.20	C
796.541	10	125542.8	4d63	5p53			1.14E+08	1.97	0.29	D+
802.832	1	124559.1	6s23	5p21			3.50E+09	0.47	0.90	C
803.010	500	124531.5	4d83	5p61			2.80E+09	0.57	0.64	C
803.806	20	124408.1	5d65	5p13			1.45E+08	1.85	0.01	D+
803.974	20	124382.1	4d41	5p73			6.16E+08	1.22	0.64	D+

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805.445	10	124155.0	4d75	5p45			7.02E+07	2.16	0.13	D+
808.568	200	D.x 123675.4	5d65	5p15			9.03E+07	2.05	0.01	D+
809.056	100	123600.8	4d57	5p25			3.76E+08	1.43	0.08	D+
809.255	50	123570.4	6s33	5p45			9.49E+09	0.03	0.72	C
810.226	200	123422.4	6s15	5p15			1.26E+10	0.09	0.92	C
810.562	1	123371.2	6s25	5p45			2.76E+09	0.57	0.98	C
812.226	1	x 123118.4	4d63	5p43			5.80E+07	2.24	0.05	D+
820.482	5	121879.6	6s23	5p33			3.80E+09	0.42	0.60	C
821.060	10	121793.8	6s13	5p11			3.04E+09	0.51	0.47	C
824.069	20	121349.1	6s11	5p31			3.31E+09	0.47	0.90	C
825.195	1000	p 121183.5	4d41	5p63			1.62E+09	0.78	0.57	C
828.279	1	120732.3	6s11	5p33			1.61E+09	0.78	0.45	C
830.886	1000	120353.5	6s13	5p25			1.03E+10	0.03	0.75	C
832.618	1000	120103.1	6s25	5p27			1.53E+10	0.20	0.98	C
834.044	5000	119897.8	4d73	5p55	834.0424	0.0018	8.56E+08	1.05	0.43	E
837.561	2000	119394.3	4d73	5p73	837.5570	0.0018	1.52E+09	0.80	0.35	C
841.738	500	118801.8	6s23	5p35			1.12E+10	0.07	0.95	C
843.194	1	118596.7	6s21	5p43			1.65E+09	0.75	0.35	C
844.072	2	118473.3	4d57	5p15			9.53E+07	1.99	0.06	D+
844.754	500	x 118377.7	4d51	5p51			2.32E+09	0.61	0.72	C
847.336	500	D.x 118016.9	5d65	5p17			1.18E+08	1.90	0.01	E
849.157	500	dc 117763.9	6s15	5p17			1.50E+10	0.21	0.96	C
849.157	500	dc 117763.9	6s31	5p83			6.86E+09	0.13	0.97	C
851.623	1	117422.9	6s33	5p63			2.66E+09	0.54	0.52	C
853.072	2	p.x 117223.4	6s25	5p63			2.54E+09	0.56	0.40	C
856.823	2	116710.2	6s21	5p41			2.72E+09	0.52	0.80	C
860.618	5000	116195.6	4d73	5p63	860.6195	0.0018	2.28E+09	0.60	0.44	C
860.800	5	116171.0	6s21	5p53			3.66E+09	0.39	0.75	C
863.029	20	115871.0	4d85	5p55	863.0271	0.0019	5.95E+08	1.17	0.18	D+
863.893	50	115755.1	6s11	5p43			3.78E+09	0.37	0.94	C
866.786	5000	115368.7	4d85	5p73	866.7907	0.0019	1.90E+09	0.66	0.39	C

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873.541	2	114476.6	6s23	5p53			1.88E+09	0.67	0.49	C
875.480	10	114223.1	6s33	5p73			4.39E+09	0.30	0.60	C
877.011	1	114023.7	6s25	5p73			1.77E+09	0.69	0.80	C
879.351	1	113720.2	6s33	5p55			1.99E+09	0.64	0.80	D
880.897	200	113520.6	6s25	5p55			7.80E+09	0.04	0.79	D
887.057	500	112732.3	4d51	5p73			6.69E+08	1.11	0.46	D+
891.516	5000	112168.5	4d85	5p63	891.5150	0.0020	3.05E+09	0.44	0.63	C
892.506	5	112044.1	6s13	5p23			3.83E+09	0.34	0.49	C
914.995	20	109290.2	4d85	5p27			3.91E+08	1.30	0.47	D+
921.000	2	108577.6	6s33	5p51			1.79E+09	0.64	0.60	C
925.122	1	108093.9	5d35	5p13			5.65E+08	1.14	0.03	D+
928.000	1	107758.6	4d41	5p43			1.24E+08	1.80	0.15	D+
938.478	5000	106555.5	4d83	5p51			2.04E+09	0.57	0.49	C
943.213	100	106020.6	4d85	5p45			3.05E+08	1.38	0.30	D+
945.016	150	105818.3	5d41	5p33			2.19E+09	0.53	0.74	C
(955.500)		A (104657.28)	4d73	5p41			1.05E+09	0.85	0.32	C
972.924	5000	102783.0	4d41	5p33			2.28E+08	1.49	0.33	D+
973.902	5	102679.7	5d31	5p11			1.21E+08	1.76	0.01	D+
983.256	50	101702.9	5d35	5p17			7.73E+07	1.95	0.04	D+
988.431	5000	101170.4	4d85	5p53			5.81E+08	1.07	0.57	D+
990.984	1000	100909.8	4d83	5p73			4.24E+08	1.20	0.19	D+
991.356	50	100871.9	4d73	5p35			4.03E+07	2.23	0.14	D+
992.272	2000	100778.8	5d25	5p13			1.82E+09	0.57	0.11	C
1009.339	200	99074.74	5d73	5p45			2.04E+09	0.51	0.64	C
1012.720	1000	98743.98	4d85	5p43			4.34E+08	1.17	0.19	D+
1017.202	500	98308.89	5d55	5p23			8.45E+08	0.89	0.03	D
1020.467	1000	97994.35	4d51	5p41			4.49E+08	1.17	0.28	D+
1021.266	200	97917.68	5s21	5p61			7.83E+07	1.91	0.03	D+
1022.554	200	97794.35	4d73	5p33			9.17E+07	1.85	0.05	D+
1023.436	2	97710.07	4d83	5p63			1.96E+07	2.51	0.01	D+
1025.821	5000	97482.89	5d75	5p45			1.07E+10	0.23	0.73	C

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_L f)$	CF	Acc.
1029.063	500	97175.78	4d73	5p31			2.53E+08	1.40	0.35	D+
1030.122	500	97075.88	5d53	5p33			1.48E+09	0.63	0.16	C
1032.576	1000	96845.17	4d85	5p35			4.39E+08	1.15	0.55	D+
1038.852	5000	96260.10	5d55	5p33			2.90E+09	0.33	0.20	C
1040.906	2000	96070.15	5d27	5p15			3.87E+09	0.20	0.36	C
1041.006	2000	96060.93	5d23	5p11			6.16E+09	0.00	0.60	C
1044.492	2000	95740.32	5d43	5p21			7.26E+09	0.08	0.47	C
1050.577	2000	95185.79	5d11	5p13			6.10E+09	0.00	0.91	C
1051.358	2000	95115.08	4d73	5p21			8.84E+07	1.84	0.09	D+
1052.487	100	95013.05	5s13	5p51			5.10E+07	2.07	0.02	D+
1053.458	500	94925.47	5d45	5p33			2.32E+09	0.41	0.24	D
1053.556	2000	94916.64	5d25	5p25			8.76E+09	0.16	0.72	C
1055.367	200	94753.77	5s15	5p55			5.68E+07	2.02	0.01	D+
1055.966	200	94700.02	5d21	5p11			3.98E+09	0.17	0.89	C
1059.473	2000	94386.55	5d25	5p17			1.03E+08	1.76	0.12	D+
1061.816	1000	94178.28	5d33	5p21			1.79E+09	0.52	0.17	C
1061.816	1000	94178.28	5d57	5p27			1.13E+10	0.28	0.78	C
1064.694	1000	93923.70	5d35	5p23			4.46E+09	0.12	0.22	C
1064.821	5000	93912.50	5d13	5p13			1.28E+10	0.34	0.88	C
1068.842	2000	93559.20	5d31	5p21			6.85E+09	0.07	0.93	C
1068.964	200	93548.52	5d33	5p23			1.05E+09	0.75	0.17	C
1072.874	5000	93207.59	5d15	5p13			1.02E+10	0.25	0.43	C
1073.192	2000	93179.97	5d13	5p15			4.58E+09	0.10	0.88	C
1074.556	1000	93061.69	5d43	5p33			5.19E+09	0.05	0.55	C
1081.130	1000	92495.81	5d17	5p15			2.21E+10	0.59	0.61	C
1081.130	1000	92495.81	5d47	5p45			3.61E+10	0.80	0.95	C
1081.395	5000	92473.15	5d15	5p15			1.65E+10	0.46	0.90	C
1084.707	500	92190.79	5d83	5p61			1.48E+10	0.42	0.94	C
1085.589	2000	92115.89	5d33	5p31			1.32E+10	0.37	0.92	C
1085.784	90	92099.35	5d53	5p43			8.62E+08	0.82	0.15	C
1088.440	2000	91874.61	5d35	5p33			1.32E+10	0.37	0.74	C

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(\text{s}^{-1})$	$\log(g_U f)$	CF	Acc.
1088.758	1000	91847.78	5d45	5p35			5.43E+09	0.02	0.59	C
1090.297	500	91718.13	4d85	5p23			3.06E+08	1.26	0.18	D+
1092.917	500	91498.26	5d31	5p31			7.50E+08	0.87	0.14	C
1094.784	500	91342.22	5s25	5p83			2.89E+08	1.29	0.30	D+
1095.491	2000	91283.27	5d55	5p43			1.30E+10	0.37	0.76	C
1097.314	5	91131.62	4d51	5p33			2.98E+07	2.28	0.06	D+
1099.589	5000	90943.07	5d27	5p25			3.23E+10	0.77	0.98	C
1100.351	1000	90880.09	5d31	5p33			9.06E+08	0.79	0.37	C
1101.745	2000	90765.10	5d11	5p11			2.82E+09	0.29	0.49	C
1104.807	200	90513.55	4d51	5p31			5.83E+07	1.98	0.16	D+
(1108.491)		B (90215.17)	5d53	5p41			1.16E+10	0.34	0.90	C
1111.222	200	89991.02	5d83	5p83			2.82E+09	0.28	0.78	C
1111.745	200	89948.68	5d45	5p43			1.34E+09	0.60	0.07	D
(1113.735)		E (89787.93)	5d65	5p63			1.13E+10	0.32	0.79	C
1114.480	2000	89727.94	5d73	5p73			7.73E+09	0.16	0.70	C
1114.688	10000	89711.20	5d19	5p17			4.43E+10	0.92	0.99	C
1115.161	1000	89673.15	5d53	5p53			1.16E+09	0.67	0.32	C
1115.532	2000	89643.33	5d29	5p27			4.44E+10	0.92	1.00	C
1116.101	1000	89597.63	5d85	5p83			2.49E+10	0.67	0.98	C
1117.413	1000	89492.43	5d13	5p11			1.66E+09	0.51	0.20	C
1118.689	2000	89390.35	5d37	5p35			3.49E+10	0.82	0.99	C
1118.987	500	89366.54	5s13	5p73			6.71E+07	1.90	0.01	D+
1125.394	2000	88857.77	5d55	5p53	D,x		5.54E+09	0.02	0.36	D+
1126.166	500	88796.86	5d35	5p35			1.19E+09	0.65	0.11	C
(1127.231)		G (88712.97)	5d51	5p73			2.14E+09	0.39	0.57	C
(1129.374)		C (88544.61)	5d63	5p63			7.98E+09	0.18	0.62	C
1134.603	2000	88136.56	5d75	5p73			1.17E+10	0.35	0.65	C
1135.257	500	88085.78	5d43	5p43			9.15E+08	0.75	0.10	C
1141.121	1000	87633.13	5d75	5p55			3.11E+09	0.22	0.33	D
1142.544	5000	87523.98	5d45	5p53			1.45E+10	0.46	0.73	C
1143.696	1000	87435.82	4d73	5p25			1.58E+07	2.51	0.04	D+

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	$\text{Unc}(\lambda_{\text{Ritz}}-\text{\AA})$	$g_U A(s^{-1})$	$\log(g_U f)$	CF	Acc.
1143.930	2000	87417.94	5d41	5p63			3.49E+09	0.16	0.57	C
1144.579	5000	87368.37	5d17	5p25			3.33E+09	0.18	0.25	C
1150.770	2000	86898.34	5d35	5p43			7.27E+09	0.16	0.67	C
1151.571	2000	86837.89	5d17	5p17			1.13E+10	0.35	0.99	C
1151.851	1000	86816.78	5d15	5p17			1.81E+09	0.45	0.83	C
1154.620	2000	86608.58	5d25	5p23			1.26E+10	0.40	0.59	C
1154.902	1000	86587.43	5d65	5p73			2.10E+09	0.38	0.21	C
1155.225	1000	86563.22	4d41	5p13			6.92E+07	1.86	0.23	D+
1158.574	2000	86313.00	5d23	5p23			6.05E+09	0.08	0.76	C
(1161.638)		F (86085.32)	5d65	5p55			8.72E+09	0.24	0.53	D+
1162.848	1000	85995.76	4d73	5p11			9.04E+07	1.75	0.08	D+
1164.083	500	85904.53	5d31	5p43			2.39E+08	1.32	0.10	D+
1167.411	2000	85659.63	5d43	5p53			2.74E+09	0.25	0.39	C
1187.404	50	84217.33	5d41	5p73		x	1.15E+09	0.61	0.81	C
(1189.322)		I (84081.49)	5d73	5p51			4.76E+09	0.04	0.74	C
1204.078	150	H,x 83051.10	5d51	5p51			4.76E+09	0.00	0.86	C
1314.039	10	76101.24	5s23	5p63			1.45E+09	0.43	0.68	C
1330.353	1	x 75168.02	5s13	5p53			7.65E+08	0.69	0.18	C
1406.536	10	71096.65	5s21	5p63			2.55E+08	1.12	0.65	D+
1411.561	5	70843.56	5s13	5p35			1.64E+08	1.31	0.02	D+
1416.418	500	70600.63	5s15	5p23			4.67E+08	0.85	0.20	C
1417.866	2000	70528.53	5s33	5p51			2.39E+09	0.14	0.84	C
1483.078	500	67427.34	5s11	5p53			4.13E+08	0.87	0.27	C
1489.263	100	67147.31	5s13	5p31			2.61E+08	1.06	0.15	C
1495.035	50	66888.07	5s11	5p41			1.55E+08	1.29	0.35	D+
1514.569	50000	66025.38	5s25	5p55			5.87E+09	0.31	0.74	D+
1521.702	10000	65715.89	5s13	5p23			2.94E+09	0.01	0.63	C
1526.201	5000	65522.17	5s25	5p73			1.39E+09	0.31	0.84	C
1529.397	5000	65385.25	5s33	5p55			1.53E+09	0.27	0.87	D
1536.037	2000	65102.60	5s23	5p53			1.04E+09	0.44	0.36	C
1538.423	5000	65001.63	5s11	5p43			2.19E+09	0.11	0.91	C

$\lambda_{\text{obs}}(\text{\AA})$	Intensity	$\sigma_{\text{obs}}(\text{cm}^{-1})$	Even level ^a	Odd level ^a	$\lambda_{\text{Ritz}}(\text{\AA})$	Unc(λ_{Ritz} , $\text{\AA}$)	$g_L A(s^{-1})$	$\log(g_L f)$	CF	Acc.
1541.255	10000	64882.19	5s33	5p73			3.10E+09	0.05	0.62	C
1548.859	2000	64563.66	5s23	5p41			1.73E+08	1.21	0.12	D+
1591.797	50000	62822.08	5s15	5p17			8.70E+09	0.52	0.97	C
1595.481	50	62677.02	5s23	5p43			2.75E+08	0.98	0.10	C
1604.549	20000	62322.81	5s25	5p63			1.63E+09	0.20	0.42	C
1605.358	10	62291.40	5s15	5p25			1.29E+08	1.30	0.06	D+
1621.198	20000	61682.78	5s33	5p63			1.28E+09	0.30	0.49	C
1621.441	20000	61673.54	5s31	5p83			3.96E+09	0.19	0.96	C
1645.331	50000	60778.04	5s23	5p35			5.80E+09	0.37	0.97	C
1663.953	50000	60097.85	5s21	5p53			2.02E+09	0.08	0.93	C
1665.978	20000	60024.80	5s11	5p33			8.35E+08	0.46	0.54	C
1679.024	20000	59558.41	5s21	5p41			1.35E+09	0.25	0.94	C
1681.349	10000	59476.05	5s31	5p61			1.84E+09	0.11	0.97	C
1682.238	50000	59444.62	5s25	5p27			7.47E+09	0.50	0.98	C
1683.307	20000	59406.87	5s11	5p31			1.48E+09	0.20	0.94	C
1724.855	1000	57975.89	5s11	5p23			6.61E+08	0.53	0.36	C
1733.090	50000	57700.41	5s23	5p33			1.77E+09	0.10	0.65	C
1733.928	50000	57672.52	5s21	5p43			1.09E+09	0.31	0.65	C
1741.944	100000	57407.13	5s13	5p25			5.00E+09	0.36	0.98	C
1749.353	50000	57163.99	5s15	5p15			4.87E+09	0.35	0.96	C
1751.844	50	57082.71	5s23	5p31			1.76E+08	1.09	0.16	C
1772.078	50000	56430.92	5s15	5p13			2.43E+09	0.06	0.92	C
1780.139	2000	56175.39	5s25	5p45			9.92E+08	0.32	0.95	C
1786.788	20000	55966.35	5s13	5p11			1.38E+09	0.19	0.95	C
1800.659	50000	55535.22	5s33	5p45			3.62E+09	0.25	0.78	C
1817.490	5000	55020.94	5s23	5p21			1.22E+09	0.22	0.96	C
1940.003	10000	51546.31	5s13	5p13			4.54E+08	0.59	0.35	C
1974.492	3	50645.94	5s21	5p23			2.04E+08	0.92	0.19	C

^aLevel codes are explained in table 2.

Symbols: dc, doubly classified; p, perturbed; u, unresolved from close line; s, shaded to shorter wavelength; l, shaded to longer wavelength; x, not included in level optimization; h, hazy
A, not observed due to break in spectrum – Ritz value

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- B, greatly perturbed by Si III line – Ritz value
- C, covered by ghost of Si IV line – Ritz value
- D, intensity much higher than expected, not used in level optimization
- E, covered by ghost of Zr V line – Ritz value
- F, covered by Si III line – Ritz value
- G, covered by ghost of Si IV line – Ritz value
- H, uncertain classification, not included in level optimization
- I, covered by neighboring strong lines – Ritz value
- J, even level for this line not included in least-squares fit

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Table 2

Odd parity energy levels (cm^{-1}) of Zr VI.

Configuration	Term	J	Design. ^a	Energy	Uncert.	No. trans. ^b
4s ² 4p ⁵	2p	3/2	p5 3	0.00	0.80	55
		1/2	p5 1	15602.78	0.97	32
4s ² 4p ⁴ 5p	³ P ₂ [1]	3/2	5p13	421257.96	0.12	20
	³ P ₂ [2]	5/2	5p15	421991.19	0.19	17
	³ P ₂ [1]	1/2	5p11	425678.16	0.18	15
	³ P ₂ [3]	5/2	5p25	427118.65	0.14	17
	³ P ₂ [3]	7/2	5p17	427649.11	0.20	13
	³ P ₁ [0]	1/2	5p21	434797.76	0.21	12
	³ P ₂ [2]	3/2	5p23	435427.69	0.15	20
	³ P ₀ [1]	1/2	5p31	436859.11	0.16	13
	³ P ₁ [2]	3/2	5p33	437477.01	0.13	26
	³ P ₁ [2]	5/2	5p35	440554.88	0.17	20
	³ P ₀ [1]	3/2	5p43	442453.66	0.15	24
	³ P ₁ [1]	1/2	5p41	444340.07	0.17	11
	³ P ₁ [1]	3/2	5p53	444879.34	0.13	20
	¹ D ₂ [3]	5/2	5p45	449730.72	0.12	16
	¹ D ₂ [3]	7/2	5p27	452999.87	0.21	10
	¹ D ₂ [1]	3/2	5p63	455878.16	0.12	19
	¹ D ₂ [2]	3/2	5p73	459077.64	0.15	20
	¹ D ₂ [2]	5/2	5p55	459580.77	0.14	15
	¹ D ₂ [1]	1/2	5p51	464724.05	0.25	9
	¹ S ₀ [1]	1/2	5p61	482699.28	0.36	6
	¹ S ₀ [1]	3/2	5p83	484897.26	0.33	8

^aDesignations are given with a short form of the configuration (two places) followed by the ordinal number of the configuration (one place) and the J value (one place). For example 5p73 indicates the seventh level with J=3/2 for the 4p⁴5p configuration. p5 3 and p5 1 indicate the J=3/2 and 1/2 levels of the 4p⁵ configuration, respectively.

n_{Total} Total number of transitions for each level, including those omitted from the level optimization procedure.

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Table 3

Even parity energy levels (cm⁻¹) of Zr VI.

Configuration	Term	J	Design.	Energy	Note ^a	Uncert.	No. trans. ^b
4s4p ⁶	2S	1/2	4p61	191570.67		0.89	8
	(³ P) ⁴ D	5/2	4d15	248940.11		0.85	6
4s ² 4p ⁴ 4d	(³ P) ⁴ D	7/2	4d17	249322.89		0.90	4
	(³ P) ⁴ D	3/2	4d13	250017.63		0.79	9
	(³ P) ⁴ D	1/2	4d11	251818.7		1.3	5
	(³ P) ⁴ F	9/2	4d19	261642.9		1.4	1
	(³ P) ⁴ F	7/2	4d27	266145.41		0.71	5
	(¹ D) ² P	1/2	4d21	266278.49		0.73	9
	(³ P) ⁴ F	3/2	4d23	271296.05		0.57	13
	(³ P) ⁴ F	5/2	4d25	271374.36		0.72	8
	(³ P) ⁴ P	1/2	4d31	272091.26		0.73	7
	(³ P) ⁴ P	3/2	4d33	272834.44		0.69	10
	(¹ D) ² D	3/2	4d43	274665.60		0.50	11
	(³ P) ² F	7/2	4d37	276491.34		0.69	6
	(³ P) ⁴ P	5/2	4d35	278742.23		0.47	10
	(¹ D) ² P	3/2	4d53	279457.21		0.41	14
	(¹ D) ² D	5/2	4d45	283112.00		0.39	12
	(¹ D) ² G	7/2	4d47	285967.09		0.65	4
	(¹ D) ² G	9/2	4d29	286411.5		1.4	1
	(³ P) ² F	5/2	4d55	287142.42		0.52	9
	(¹ D) ² F	5/2	4d65	299608.66		0.45	9
	(¹ D) ² F	7/2	4d57	303517.22		0.48	6
	(¹ S) ² D	3/2	4d63	319336.18		0.60	8
	(¹ S) ² D	5/2	4d75	325576.82		0.75	4
	(¹ D) ² S	1/2	4d41	334694.92		0.33	7
	(³ P) ² P	3/2	4d73	339682.78		0.21	11
	(³ P) ² D	5/2	4d85	343709.55		0.22	11

Configuration	Term	J	Design.	Energy	Note ^a	Uncert.	No. trans. ^b
4s ² 4p ⁴ 5s	(³ P) ² P	1/2	4d51	346345.56		0.42	7
	(³ P) ² D	3/2	4d83	358168.09		0.32	7
	(³ P ₂)[2]	5/2	5s15	364827.11		0.12	7
	(³ P ₂)[2]	3/2	5s13	369711.65		0.11	11
	(³ P ₀)[0]	1/2	5s11	377452.05		0.12	8
	(³ P ₁)[1]	3/2	5s23	379776.65		0.11	10
	(³ P ₁)[1]	1/2	5s21	384781.44		0.16	8
	(¹ D ₂)[2]	5/2	5s25	393555.34		0.11	7
	(¹ D ₂)[2]	3/2	5s33	394195.47		0.11	7
	(¹ S ₀)[0]	1/2	5s31	423223.46		0.33	4
4s ² 4p ⁴ 5d	(³ P ₂)[2]	5/2	5d15	514465.31		0.46	3
	(³ P ₂)[3]	7/2	5d17	514487.01		0.30	3
	(³ P ₂)[2]	3/2	5d13	515170.73		0.31	4
	(³ P ₂)[1]	1/2	5d11	516443.48		0.37	2
	(³ P ₂)[4]	9/2	5d19	517360.31	*	0.45	1
				517292.44	#	0.45	1
	(³ P ₂)[4]	7/2	5d27	518061.55		0.35	2
	(³ P ₂)[0]	1/2	5d21	520378.18	*	0.48	2
	(³ P ₂)[1]	3/2	5d23	521740.06		0.63	4
	(³ P ₂)[3]	5/2	5d25	522035.99		0.34	5
	(³ P ₁)[1]	1/2	5d31	528357.52		0.31	7
	(³ P ₀)[2]	3/2	5d33	528976.13		0.44	4
	(³ P ₀)[2]	5/2	5d35	529351.71		0.24	7
	(³ P ₁)[3]	7/2	5d37	529945.22		0.43	1
	(³ P ₁)[1]	3/2	5d43	530538.91		0.37	6
	(³ P ₁)[2]	5/2	5d45	532402.86		0.34	5
	(³ P ₁)[3]	5/2	5d55	533736.95		0.25	5

Configuration	Term	J	Design.	Energy	Note ^a	Uncert.	No. trans. ^b
4s ² 4p ⁴ 6s	(³ P ₁) 2]	3/2	5d53	534552.78		0.29	6
	(¹ D ₂) 4]	7/2	5d47	542226.54	*	0.45	1
	(¹ D ₂) 4]	9/2	5d29	542643.20	*	0.45	1
				542711.07	#	0.45	1
	(¹ D ₂) 0]	1/2	5d41	543295.84		0.41	5
	(¹ D ₂) 1]	3/2	5d63	544423		10	2
	(¹ D ₂) 2]	5/2	5d65	545666.07		0.78	5
	(¹ D ₂) 3]	7/2	5d57	547178.00	*	0.50	0
	(¹ D ₂) 3]	5/2	5d75	547213.94		0.28	4
	(¹ D ₂) 1]	1/2	5d51	547791		11	3
	(¹ D ₂) 2]	3/2	5d73	548805.54		0.33	4
	(¹ S ₀) 2]	5/2	5d85	574494.88		0.52	2
	(¹ S ₀) 2]	3/2	5d83	574889.14		0.74	3
	(³ P ₂) 2]	5/2	6s15	545413.52		0.77	3
	(³ P ₂) 2]	3/2	6s13	547471.92		0.42	5
	(³ P ₀) 0]	1/2	6s11	558208.73		0.48	4
	(³ P ₁) 1]	3/2	6s23	559356.47		0.41	6
	(³ P ₁) 1]	1/2	6s21	561050.32		0.41	5
	(¹ D ₂) 2]	5/2	6s25	573101.84		0.48	6
	(¹ D ₂) 2]	3/2	6s33	573301.14		0.35	6
	(¹ S ₀) 0]	1/2	6s31	602661.0		4.0	3

^aDesignations are explained in table 2; 4p61 indicates the ²S_{1/2} level of 4s4p⁶.

^bTotal number of transitions for each level, including those omitted from the level optimization procedure.

Notes:

* Tentative value; not included in least-squares fit

Alternate value for interchange of classifications of λ1114.688 and 1115.532 Å

Hartree-Fock and least-squares fitted parameters (cm⁻¹) for the odd configurations of Zr VI. Mean error of fit 229 cm⁻¹.

Table 4

Configuration	Parameter	HFR	LSF	Unc.	LSF/HFR
4s ² 4p ⁵	E _{av} (4s ² 4p ⁵)	9676	9927	172	
	ζ _{4p}	9986	10481	217	1.049
4s ² 4p ⁴ 5p	E _{av} (4s ² 4p ⁴ 5p)	448691	443928	52	0.989
	F ² (4p4p)	84030	69669	504	0.829
	α(4p4p)		-59 ^a		
	ζ _{4p}	10556	10858	133	1.031
	ζ _{5p}	2371	2725	108	1.148
	F ² (4p5p)	26016	24044	484	0.924
Config. Interaction	G ⁰ (4p5p)	5518	4725	62 ^b	0.856
	G ² (4p5p)	7441	6372	84 ^b	0.856
	4s ² 4p ⁵ -4s ² 4p ⁴ 5p	2417	2054 ^c		0.850
	R ² (4p4p,4p5p)	11574	9837 ^c		0.850

^aFixed at value from 4p⁴ of Zr VII [15].

^bLinked in LSF fit.

^cFixed at scaled HFR value.

Table 5

Calculated energy levels (cm^{-1}) and percentage compositions for the odd levels of Zr VI.

J	Observed	Calculated	O-C	%Jl	Percentage Composition (LS-coupling)	
3/2	0	0	0		99%	$4s^2 4p^5 (^1S)^2P$
1/2	15603	15603	0		99%	$4s^2 4p^5 (^1S)^2P$
3/2	421258	421351	-93	40% (3P_2)[1]	63%	$4p^4 5p (^3P)^4P$
5/2	421991	421956	36	79% (3P_2)[2]	68%	$4p^4 5p (^3P)^4P$
1/2	425678	426061	-383	54% (3P_2)[1]	44%	$4p^4 5p (^3P)^4P$
5/2	427119	427158	-40	73% (3P_2)[3]	60%	$4p^4 5p (^3P)^2D$
7/2	427649	427446	203	90% (3P_2)[3]	90%	$4p^4 5p (^3P)^4D$
1/2	434798	434708	89	55% (3P_1)[0]	38%	$4p^4 5p (^3P)^4P$
3/2	435428	435079	348	35% (3P_2)[2]	33%	$4p^4 5p (^3P)^4D$
1/2	436859	436807	52	57% (3P_0)[1]	56%	$4p^4 5p (^3P)^4D$
3/2	437477	437528	-51	35% (3P_1)[2]	49%	$4p^4 5p (^3P)^4D$
5/2	440555	440408	147	96% (3P_1)[2]	60%	$4p^4 5p (^3P)^4D$
3/2	442454	442494	-40	67% (3P_0)[1]	25%	$4p^4 5p (^3P)^2D$
3/2	444879	444863	17	64% (3P_1)[1]	44%	$4p^4 5p (^3P)^2D$
1/2	444340	444928	-587	63% (3P_1)[1]	68%	$4p^4 5p (^3P)^2S$
5/2	449731	449565	166	84% (1D_2)[3]	84%	$4p^4 5p (^1D)^2F$
7/2	453000	452862	138	89% (1D_2)[3]	89%	$4p^4 5p (^1D)^2F$
3/2	455878	455924	-46	58% (1D_2)[1]	58%	$4p^4 5p (^1D)^2P$
3/2	459078	458938	139	71% (1D_2)[2]	71%	$4p^4 5p (^1D)^2D$
5/2	459581	459514	67	90% (1D_2)[2]	90%	$4p^4 5p (^1D)^2D$
1/2	464724	464776	-52	62% (1D_2)[1]	62%	$4p^4 5p (^1D)^2P$
1/2	482699	482755	-56	79% (1S_0)[1]	79%	$4p^4 5p (^1S)^2P$
3/2	484897	484952	-55	81% (1S_0)[1]	81%	$4p^4 5p (^1S)^2P$
					4%	$4p^4 5p (^3P)^4D$
					17%	$4p^4 5p (^3P)^2P$
					18%	$4p^4 5p (^3P)^2P$
					15%	$4p^4 5p (^3P)^2S$
					10%	$4p^4 5p (^1D)^2P$
					14%	$4p^4 5p (^3P)^4P$
					17%	$4p^4 5p (^3P)^4P$
					5%	$4p^4 5p (^3P)^4P$
					10%	$4p^4 5p (^3P)^4D$
					4%	$4p^4 5p (^1D)^2D$
					10%	$4p^4 5p (^3P)^2P$
					8%	$4p^4 5p (^1D)^2P$
					3%	$4p^4 5p (^3P)^4P$
					2%	$4p^4 5p (^1S)^2P$
					6%	$4p^4 5p (^3P)^4D$
					4%	$4p^4 5p (^3P)^4D$

Table 6

Hartree-Fock and least-squares fitted parameters (cm^{-1}) for the even configurations of Zr VI. Mean error of fit 303 cm^{-1} .

Configuration	Parameter	HF	LSF	Unc.	LSF/HFR
4s4p ⁶	$E_{av}(4s4p^6)$	238204	225794	545	0.945
	$E_{av}(4s^24p^44d)$	291306	286394	61	0.982
4s ² 4p ⁴ 4d	$F^2(4p4p)$	82691	68538	720	0.829
	$\alpha(4p4p)$		-59 ^a		
	ζ_{4p}	10169	10463	168	1.029
	ζ_{4d}	719	853	81	1.186
	$F^2(4p4d)$	69587	60676	549	0.872
	$G^1(4p4d)$	86663	69960	180	0.807
	$G^3(4p4d)$	53745	45371	1036	0.844
	$E_{av}(4s^24p^45s)$	388500	383302	110	0.986
	$F^2(4p4p)$	83691	69792	1010	0.834
	$\alpha(4p4p)$		-59 ^a		
4s ² 4p ⁴ 5d	ζ_{4p}	10481	10832	274	1.033
	$G^1(4p5s)$	8701	7486	414	0.860
	$E_{av}(4s^24p^45d)$	538379	533803	70	0.991
	$F^2(4p4p)$	84085	70231	594	0.835
	$\alpha(4p4p)$		-59 ^a		
	ζ_{4p}	10550	10927	141	1.036
	ζ_{5d}	217	274	76	1.265
	$F^2(4p5d)$	19526	16999	721	0.871
	$G^1(4p5d)$	10862	7658 ^b	275	0.705
	$G^3(4p5d)$	8028	5660 ^b	203	0.705
4s ² 4p ⁴ 6s	$E_{av}(4s^24p^46s)$	566615	562487	112	0.992
	$F^2(4p4p)$	84157	69956	914	0.831
	$\alpha(4p4p)$		-59 ^a		
	ζ_{4p}	10581	11023	237	1.042

Configuration	Parameter	HF	LSF	Unc.	LSF/HFR
Config. interaction					
	$G^1(4p6s)$	2783	2415	380	0.868
$4s4p^6-4s^24p^44d$	$R^1(4p4p,4s4d)$	95949	74285 ^c	461	0.774
$4s4p^6-4s^24p^45d$	$R^1(4p4p,4s5d)$	32261	24977 ^c	155	0.774
$4s4p^6-4s^24p^45s$	$R^1(4p4p,4s5s)$	3749	3186 ^d		0.850
$4s4p^6-4s^24p^46s$	$R^1(4p4p,4s6s)$	875	744 ^d		0.850
$4s^24p^44d-4s^24p^45s$	$R^2(4p4d,4p5s)$	-8467	-7197 ^d		0.850
	$R^1(4p4d,5s4p)$	-1073	-912 ^d		0.850
$4s^24p^44d-4s^24p^46s$	$R^2(4p4d,4p6s)$	-5150	-4378 ^d		0.850

^a fixed at value from $4p^4$ of Zr VII [15]

^{b, c} linked in groups in LSF fit

^d fixed at scaled HFR value.

Table 7

Calculated energy levels (cm^{-1}) and percentage compositions for the even levels of Zr VI. Observed levels with asterisk were not included in the least-squares fits.

J	Observed	Calculated	O-C	% <i>Jl</i>	Percentage Composition (LS-coupling)				
1/2	191571	191569	2	77%	4s4p(² S) ² S	23%	4p ⁴ 4d(¹ D) ² S		
5/2	248940	248803	137	88%	4p ⁴ 4d(³ P) ⁴ D	3%	4p ⁴ 4d(³ P) ⁴ F	3%	4p ⁴ 4d(³ P) ⁴ P
7/2	249323	249305	18	91%	4p ⁴ 4d(³ P) ⁴ D	6%	4p ⁴ 4d(³ P) ⁴ F	2%	4p ⁴ 4d(¹ D) ² F
3/2	250018	249861	157	86%	4p ⁴ 4d(³ P) ⁴ D	4%	4p ⁴ 4d(³ P) ⁴ P	3%	4p ⁴ 4d(¹ D) ² D
1/2	251819	251854	-35	85%	4p ⁴ 4d(³ P) ⁴ D	7%	4p ⁴ 4d(¹ D) ² P	5%	4p ⁴ 4d(³ P) ² P
9/2	261643	261550	93	90%	4p ⁴ 4d(³ P) ⁴ F	10%	4p ⁴ 4d(¹ D) ² G		
7/2	266145	265981	164	66%	4p ⁴ 4d(³ P) ⁴ F	17%	4p ⁴ 4d(³ P) ² F	13%	4p ⁴ 4d(¹ D) ² G
1/2	266279	267364	-1085	44%	4p ⁴ 4d(¹ D) ² P	37%	4p ⁴ 4d(³ P) ² P	14%	4p ⁴ 4d(³ P) ⁴ D
3/2	271296	271001	295	47%	4p ⁴ 4d(³ P) ⁴ F	16%	4p ⁴ 4d(³ P) ⁴ P	13%	4p ⁴ 4d(¹ S) ² D
5/2	271374	271025	349	93%	4p ⁴ 4d(³ P) ⁴ F	3%	4p ⁴ 4d(³ P) ⁴ D	2%	4p ⁴ 4d(¹ S) ² D
1/2	272091	272034	57	91%	4p ⁴ 4d(³ P) ⁴ P	5%	4p ⁴ 4d(³ P) ² P	3%	4p ⁴ 4d(¹ D) ² P
3/2	272834	272884	-50	38%	4p ⁴ 4d(³ P) ⁴ P	30%	4p ⁴ 4d(³ P) ⁴ F	18%	4p ⁴ 4d(¹ D) ² P
3/2	274666	274573	93	36%	4p ⁴ 4d(¹ D) ² D	21%	4p ⁴ 4d(³ P) ² D	15%	4p ⁴ 4d(³ P) ⁴ F
7/2	276491	276813	-322	42%	4p ⁴ 4d(³ P) ² F	25%	4p ⁴ 4d(³ P) ⁴ F	20%	4p ⁴ 4d(¹ D) ² G
5/2	278742	278634	108	74%	4p ⁴ 4d(³ P) ⁴ P	9%	4p ⁴ 4d(¹ S) ² D	7%	4p ⁴ 4d(³ P) ² D
3/2	279457	279886	-429	40%	4p ⁴ 4d(³ P) ⁴ P	24%	4p ⁴ 4d(¹ D) ² P	22%	4p ⁴ 4d(³ P) ² P
5/2	283112	282808	304	41%	4p ⁴ 4d(¹ D) ² D	21%	4p ⁴ 4d(³ P) ² D	18%	4p ⁴ 4d(³ P) ⁴ P
7/2	285967	285629	338	65%	4p ⁴ 4d(¹ D) ² G	24%	4p ⁴ 4d(³ P) ² F	10%	4p ⁴ 4d(¹ D) ² F
9/2	286412	285935	477	90%	4p ⁴ 4d(¹ D) ² G	10%	4p ⁴ 4d(³ P) ⁴ F		
5/2	287142	287795	-653	65%	4p ⁴ 4d(³ P) ² F	21%	4p ⁴ 4d(¹ D) ² F	9%	4p ⁴ 4d(¹ D) ² D
5/2	299609	299713	-104	76%	4p ⁴ 4d(¹ D) ² F	13%	4p ⁴ 4d(³ P) ² F	9%	4p ⁴ 4d(¹ D) ² D
7/2	303517	303641	-124	80%	4p ⁴ 4d(¹ D) ² F	17%	4p ⁴ 4d(³ P) ² F	2%	4p ⁴ 4d(¹ D) ² G
3/2	319336	319335	1	63%	4p ⁴ 4d(¹ S) ² D	25%	4p ⁴ 4d(¹ D) ² D	5%	4p ⁴ 4d(¹ D) ² P
5/2	325577	325582	-5	73%	4p ⁴ 4d(¹ S) ² D	14%	4p ⁴ 4d(¹ D) ² D	5%	4p ⁴ 4d(³ P) ² F
1/2	334695	334774	-79	69%	4p ⁴ 4d(¹ D) ² S	20%	4s4p6(² S) ² S	5%	4p ⁴ 4d(¹ D) ² P
3/2	339683	339272	411	50%	4p ⁴ 4d(³ P) ² P	36%	4p ⁴ 4d(¹ D) ² P	7%	4p ⁴ 4d(¹ D) ² D

J	Observed	Calculated	O-C	% <i>J_L</i>	Percentage Composition (LS-coupling)					
5/2	343710	344309	-599		64%	4p ⁴ 4d(3p) ² D	21%	4p ⁴ 4d(1D) ² D	11%	4p ⁴ 4d(1S) ² D
1/2	346346	345581	764		48%	4p ⁴ 4d(3p) ² P	41%	4p ⁴ 4d(1D) ² P	7%	4p ⁴ 4d(1D) ² S
3/2	358168	358453	-285		57%	4p ⁴ 4d(3p) ² D	19%	4p ⁴ 4d(1S) ² D	14%	4p ⁴ 4d(1D) ² D
5/2	364827	364804	23	92% (3P ₂)[2]	92%	4p ⁴ 5s(3p) ⁴ P	8%	4p ⁴ 5s(1D) ² D		
3/2	369712	369708	4	82% (3P ₂)[2]	51%	4p ⁴ 5s(3p) ² P	38%	4p ⁴ 5s(3p) ⁴ P	10%	4p ⁴ 5s(1D) ² D
1/2	377452	377471	-19	63% (3P ₀)[0]	90%	4p ⁴ 5s(3p) ⁴ P	9%	4p ⁴ 5s(1S) ² S		
3/2	379777	379741	36	92% (3P ₁)[1]	61%	4p ⁴ 5s(3p) ⁴ P	37%	4p ⁴ 5s(3p) ² P	2%	4p ⁴ 5s(1D) ² D
1/2	384781	384780	1	72% (3P ₁)[1]	94%	4p ⁴ 5s(3p) ² P	5%	4p ⁴ 5s(1S) ² S	1%	4p ⁴ 5s(3p) ⁴ P
5/2	393555	393590	-35	92% (1D ₂)[2]	92%	4p ⁴ 5s(1D) ² D	8%	4p ⁴ 5s(3p) ⁴ P		
3/2	394196	394238	-42	87% (1D ₂)[2]	87%	4p ⁴ 5s(1D) ² D	12%	4p ⁴ 5s(3p) ² P	1%	4p ⁴ 5s(3p) ⁴ P
1/2	423224	423190	34	85% (1S ₀)[0]	85%	4p ⁴ 5s(1S) ² S	8%	4p ⁴ 5s(3p) ⁴ P	6%	4p ⁴ 5s(3p) ² P
5/2	514465	514521	-56	55% (3P ₂)[2]	70%	4p ⁴ 5d(3p) ⁴ D	10%	4p ⁴ 5d(3p) ⁴ F	10%	4p ⁴ 5d(3p) ⁴ P
7/2	514487	514569	-82	91% (3P ₂)[3]	73%	4p ⁴ 5d(3p) ⁴ D	19%	4p ⁴ 5d(3p) ⁴ F	6%	4p ⁴ 5d(1D) ² F
3/2	515171	515206	-35	61% (3P ₂)[2]	59%	4p ⁴ 5d(3p) ⁴ D	20%	4p ⁴ 5d(3p) ⁴ P	6%	4p ⁴ 5d(1D) ² D
1/2	516444	516516	-72	77% (3P ₂)[1]	43%	4p ⁴ 5d(3p) ⁴ D	27%	4p ⁴ 5d(3p) ⁴ P	17%	4p ⁴ 5d(3p) ² P
9/2	517360	*	517149	90% (3P ₂)[4]	90%	4p ⁴ 5d(3p) ⁴ F	10%	4p ⁴ 5d(1D) ² G		
7/2	518062	517900	162	87% (3P ₂)[4]	65%	4p ⁴ 5d(3p) ² F	22%	4p ⁴ 5d(3p) ⁴ F	11%	4p ⁴ 5d(1D) ² G
1/2	520378	*	520366	82% (3P ₂)[0]	53%	4p ⁴ 5d(3p) ⁴ P	29%	4p ⁴ 5d(3p) ² P	11%	4p ⁴ 5d(1D) ² S
3/2	521740	521749	-9	65% (3P ₂)[1]	37%	4p ⁴ 5d(3p) ⁴ P	34%	4p ⁴ 5d(3p) ² D	13%	4p ⁴ 5d(3p) ² P
5/2	522036	521991	45	54% (3P ₂)[3]	40%	4p ⁴ 5d(3p) ² D	24%	4p ⁴ 5d(3p) ² F	15%	4p ⁴ 5d(3p) ⁴ P
1/2	528358	528514	-156	88% (3P ₁)[1]	53%	4p ⁴ 5d(3p) ⁴ D	30%	4p ⁴ 5d(3p) ² P	9%	4p ⁴ 5d(3p) ⁴ P
3/2	528976	528938	38	68% (3P ₀)[2]	69%	4p ⁴ 5d(3p) ⁴ F	12%	4p ⁴ 5d(3p) ⁴ D	11%	4p ⁴ 5d(1S) ² D
5/2	529352	529301	51	52% (3P ₀)[2]	59%	4p ⁴ 5d(3p) ⁴ F	14%	4p ⁴ 5d(3p) ⁴ D	13%	4p ⁴ 5d(3p) ⁴ P
7/2	529945	529891	54	97% (3P ₁)[3]	54%	4p ⁴ 5d(3p) ⁴ F	23%	4p ⁴ 5d(3p) ² F	22%	4p ⁴ 5d(3p) ⁴ D
3/2	530539	530479	60	59% (3P ₁)[1]	28%	4p ⁴ 5d(3p) ⁴ P	26%	4p ⁴ 5d(3p) ⁴ D	19%	4p ⁴ 5d(3p) ² D
5/2	532403	532272	131	97% (3P ₁)[2]	52%	4p ⁴ 5d(3p) ⁴ P	27%	4p ⁴ 5d(3p) ² F	11%	4p ⁴ 5d(3p) ⁴ F
5/2	533737	533656	81	59% (3P ₁)[3]	43%	4p ⁴ 5d(3p) ² D	42%	4p ⁴ 5d(3p) ² F	4%	4p ⁴ 5d(1S) ² D
3/2	534553	534777	-224	46% (3P ₁)[2]	64%	4p ⁴ 5d(3p) ² P	17%	4p ⁴ 5d(3p) ² D	7%	4p ⁴ 5d(1D) ² P

J	Observed	Calculated	O-C	% <i>Jl</i>	Percentage Composition (LS-coupling)						
7/2	542227	*	542081	146	88% (¹ D ₂)[4]	88%	4p ⁴ 5d(¹ D) ² G	8%	4p ⁴ 5d(³ P) ² F	3%	4p ⁴ 5d(³ P) ⁴ F
9/2	542643	*	542576	67	90% (¹ D ₂)[4]	90%	4p ⁴ 5d(¹ D) ² G	10%	4p ⁴ 5d(³ P) ⁴ F		
1/2	543296		543203	93	79% (¹ D ₂)[0]	79%	4p ⁴ 5d(¹ D) ² S	10%	4p ⁴ 5d(³ P) ⁴ P	9%	4p ⁴ 5d(¹ D) ² P
3/2	544423		544296	127	76% (¹ D ₂)[1]	76%	4p ⁴ 5d(¹ D) ² P	7%	4p ⁴ 5d(³ P) ⁴ P	6%	4p ⁴ 6s(³ P) ² P
5/2	545413		545437	-23	91% (³ P ₂)[2]	91%	4p ⁴ 6s(³ P) ⁴ P	9%	4p ⁴ 6s(¹ D) ² D		
5/2	545666		545709	-43	76% (¹ D ₂)[2]	76%	4p ⁴ 5d(¹ D) ² D	17%	4p ⁴ 5d(¹ D) ² F	2%	4p ⁴ 5d(³ P) ⁴ D
5/2	547214		547087	127	73% (¹ D ₂)[3]	73%	4p ⁴ 5d(¹ D) ² F	15%	4p ⁴ 5d(¹ D) ² D	7%	4p ⁴ 5d(³ P) ² D
3/2	547472		547461	11	82% (³ P ₂)[2]	63%	4p ⁴ 6s(³ P) ² P	20%	4p ⁴ 6s(³ P) ⁴ P	9%	4p ⁴ 6s(¹ D) ² D
7/2	547178	*	547229	-51	92% (¹ D ₂)[3]	92%	4p ⁴ 5d(¹ D) ² F	3%	4p ⁴ 5d(³ P) ⁴ D	2%	4p ⁴ 5d(³ P) ² F
1/2	547791		547844	-53	67% (¹ D ₂)[1]	67%	4p ⁴ 5d(¹ D) ² P	23%	4p ⁴ 5d(³ P) ² P	8%	4p ⁴ 5d(¹ D) ² S
3/2	548806		549016	-210	78% (¹ D ₂)[2]	78%	4p ⁴ 5d(¹ D) ² D	18%	4p ⁴ 5d(³ P) ² D	1%	4p ⁴ 5d(¹ D) ² P
1/2	558209		558212	-3	70% (³ P ₀)[0]	86%	4p ⁴ 6s(³ P) ⁴ P	12%	4p ⁴ 6s(¹ S) ² S	2%	4p ⁴ 6s(³ P) ² P
3/2	559357		559340	17	99% (³ P ₁)[1]	78%	4p ⁴ 6s(³ P) ⁴ P	22%	4p ⁴ 6s(³ P) ² P		
1/2	561050		561077	-27	81% (³ P ₁)[1]	92%	4p ⁴ 6s(³ P) ² P	4%	4p ⁴ 6s(³ P) ⁴ P	3%	4p ⁴ 6s(¹ S) ² S
5/2	573102		573108	-6	91% (¹ D ₂)[2]	91%	4p ⁴ 6s(¹ D) ² D	9%	4p ⁴ 6s(³ P) ⁴ P		
3/2	573301		573265	36	88% (¹ D ₂)[2]	88%	4p ⁴ 6s(¹ D) ² D	9%	4p ⁴ 6s(³ P) ² P	2%	4p ⁴ 5d(¹ S) ² D
5/2	574495		574483	12	85% (¹ S ₀)[2]	85%	4p ⁴ 5d(¹ S) ² D	4%	4p ⁴ 5d(³ P) ² F	3%	4p ⁴ 5d(³ P) ⁴ P
3/2	574889		574920	-31	81% (¹ S ₀)[2]	81%	4p ⁴ 5d(¹ S) ² D	6%	4p ⁴ 5d(³ P) ⁴ F	4%	4p ⁴ 5d(³ P) ² D
1/2	602660		602671	-11	85% (¹ S ₀)[0]	85%	4p ⁴ 6s(¹ S) ² S	9%	4p ⁴ 6s(³ P) ⁴ P	5%	4p ⁴ 6s(³ P) ² P

Table 8

Comparison of wavelengths $\lambda(\text{\AA})$ and transition probabilities $A(\text{s}^{-1})$ for Zr VI calculated with the MCDF2 method of Singh et al. [18] and the GRASP3 method of Aggarwal and Keenan [19] with present values. Numerals following level names are index numbers used in [18] and [19]. Blank spaces indicate that line was not observed. Acc. is the accuracy estimate.

Lower level	Upper level	$\lambda[18]$	$\lambda[19]$	$\lambda(\text{pres.})$	$A[18]$	$A[19]$	$A(\text{pres.})$	CF	Acc.	Int.(obs)
$4s^2 4p^5 \ ^2P_{3/2}$ 1	$4s 4p^6 \ ^2S_{1/2}$ 3	528	494.113	522.000	5.30E+08	1.0518E+09	1.31E+09	0.04	D+	2000
	$4s^2 4p^4 4d \ (^3P)^4D_{5/2}$ 4	410	392.117	401.701	1.17E+07	2.0308E+07	9.49E+06	0.00	E	80
	$(^3P)^4D_{3/2}$ 6	408	390.213	399.967	7.76E+06	1.1017E+07	1.22E+07	0.00	E	80
	$(^3P)^4D_{1/2}$ 7	405	387.245	397.112	4.75E+06	5.6982E+06	1.40E+07	0.01	E	30
	$(^1D)^2P_{1/2}$ 10	376	359.833	375.546	1.28E+07	2.1200E+08	1.49E+07	0.00	E	30
	$(^3P)^4F_{3/2}$ 12	372	359.150	368.600	3.35E+05	5.1086E+05	2.13E+08	0.01	D+	250
	$(^3P)^4F_{5/2}$ 11	374	360.799	368.494	1.41E+08	1.0789E+07	2.14E+08	0.61	D+	300
	$(^3P)^4P_{1/2}$ 13	368	353.993	367.523	4.67E+08	5.9759E+08	8.61E+08	0.15	D+	300
	$(^3P)^4P_{3/2}$ 14	368	353.991	366.522	5.50E+08	7.0038E+08	5.27E+08	0.02	D+	200
	$(^1D)^2D_{3/2}$ 15	365	351.232	364.080	3.37E+08	2.5390E+08	3.80E+08	0.01	D+	300
	$(^3P)^4P_{5/2}$ 17	360	346.875	358.755	1.60E+08	1.5603E+08	2.85E+08	0.02	D+	300
	$(^1D)^2P_{3/2}$ 18	358	344.980	357.837	6.97E+07	1.7608E+07	5.52E+07	0.00	D+	30
	$(^1D)^2D_{5/2}$ 19	354	340.992	353.221	3.82E+08	2.6359E+08	4.00E+08	0.01	D+	250
	$(^3P)^2F_{5/2}$ 22	348	335.698	348.262	1.96E+08	3.0306E+08	1.56E+08	0.01	D+	200p
	$(^1D)^2F_{5/2}$ 23	330	318.897	333.768	3.24E+08	3.9608E+08	4.95E+08	0.10	D+	400
	$(^1S)^2D_{3/2}$ 25	306	304.453	313.150	1.68E+09	4.0018E+09	3.18E+09	0.11	D+	300
	$(^1S)^2D_{5/2}$ 26	301	300.149	307.148	3.16E+02	2.1104E+09	5.26E+05	0.00	E	30
	$(^1D)^2S_{1/2}$ 28	279	280.532	298.779	1.63E+11	9.7116E+10	1.41E+11	0.71	C	300
	$(^3P)^2P_{3/2}$ 27	281	283.619	294.395	1.56E+11	1.2527E+11	1.46E+11	0.90	C	500
	$(^3P)^2D_{5/2}$ 30	274	277.998	290.949	1.29E+10	1.6154EE11	1.75E+11	0.85	C	500
	$(^3P)^2P_{1/2}$ 29	275	273.019	288.730	1.91E+11	6.3978E+10	1.38E+10	0.11	D+	200
	$(^3P)^2D_{3/2}$ 31	265	268.277	279.198	7.17E+09	7.1045E+09	4.46E+09	0.05	D+	90p
$4s^2 4p^5 \ ^2P_{1/2}$ 2	$4s 4p^6 \ ^2S_{1/2}$ 3	574	534.239	568.284	2.40E+08	4.7253E+08	5.97E+08	0.05	D+	2000

Lower level	Upper level	$\lambda[18]$	$\lambda[19]$	$\lambda(\text{pres.})$	A[18]	A[19]	A(pres.)	[CF]	Acc.	Int.(obs)
$4s^2 4p^4 4d$ (3P) $^4D_{3/2}$	6	435	414.818		3.21E+05	1.2890E+00	2.31E+06	0.00	E	
	7	431	411.465	423.344	4.55E+06	4.8266E+06	9.63E+06	0.00	E	5
	10	398	380.653	398.919	6.32E+07	6.0598E+07	7.66E+07	0.00	E	80
	12	395	379.890	391.094	3.56E+07	5.1666E+07	9.18E+06	0.00	E	100p
	13	390	374.124	389.881	2.37E+07	2.6970E+07	7.14E+07	-0.01	E	100p
	14	390	374.122	388.754	1.58E+07	3.2332E+06	8.46E+06	0.00	E	20
	15	386	371.042	386.007	3.78E+08	4.0027E+08	3.88E+08	-0.01	D+	250
	18	379	364.072	378.992	2.06E+07	1.1180E+07	1.51E+07	0.00	E	80
	25	321	319.226	329.242	2.20E+09	6.9689E+08	3.28E+09	-0.06	D+	300
	28	291	293.028	313.389	8.16E+09	3.9101E+10	1.27E+10	-0.11	C	300
	27	294	296.397	308.569	3.20E+09	2.5940E+09	1.16E+09	0.02	D+	100
	29	286	284.840	302.351	1.52E+11	9.6829E+10	1.28E+11	-0.87	C	300
	31	276	279.682	291.920	1.80E+11	1.5364E+11	1.65E+11	0.85	C	500p

Table 9

Comparison of level energies $E(\text{cm}^{-1})$ for Zr VI calculated with the MCDF2 method of Singh et al. [18] and the GRASP3 method of Aggarwal and Keenan [19] with present experimental energies. Index numbers are those used in [18] and [19].

Configuration	Term	J	Index	E[18]	E[19]	E(present)
$4s^2 4p^5$	$2p$	3/2	1	0	0.00	0.00
	$2p$	1/2	2	15132.68	15200.72	15602.78
$4s 4p^6$	$2s$	1/2	3	189416.50	202382.92	191570.67
	$(^3P^4D)$	5/2	4	243856.87	255025.79	248940.11
$4s^2 4p^4 4d$	$(^3P^4D)$	7/2	5	243977.58	255226.61	249322.89 ^a
	$(^3P^4D)$	3/2	6	245129.81	256270.21	250017.63
	$(^3P^4D)$	1/2	7	247050.21	258234.49	251818.7 ^a
	$(^3P^4F)$	9/2	8	257617.85	268478.41	261642.9 ^a
	$(^3P^4F)$	7/2	9	262852.29	273655.78	266145.41
	$(^1D)^3P$	1/2	10	266287.05	277906.98	266278.49
	$(^3P^4F)$	3/2	12	267351.49	278434.81	271296.05
	$(^3P^4F)$	5/2	11	268547.62	277162.97	271374.36
	$(^3P^4P)$	1/2	13	271422.72	282491.78	272091.26
	$(^3P^4P)$	3/2	14	271795.83	282492.88	272834.44
	$(^1D)^3D$	3/2	15	274341.72	284711.75	274665.60
	$(^3P^2F)$	7/2	16	275087.93	285754.25	276491.34 ^a
	$(^3P^4P)$	5/2	17	278072.77	288288.07	278742.23
	$(^1D)^3P$	3/2	18	279170.13	289871.57	279457.21
	$(^1D)^3D$	5/2	19	282736.58	293262.43	283112.00
	$(^1D)^3G$	7/2	20	285041.05	295528.49	285967.09 ^a
	$(^1D)^3G$	9/2	21	285304.42	295244.28	286411.5
	$(^3P^2F)$	5/2	22	287334.54	297886.73	287142.42
	$(^1D)^3F$	5/2	23	303235.39	313598.83	299608.66
	$(^1D)^3F$	7/2	24	306845.73	317300.25	303517.22
	$(^1S)^3D$	3/2	25	327037.28	328458.27	319336.18

Configuration	Term	J	Index	E[18]	E[19]	E(present)
	(¹ S) ² D	5/2	26	332337.56	333168.17	325576.82 ^a
	(¹ D) ² S	1/2	28	358608.52	356465.26	334694.92
	(³ P) ² P	3/2	27	355733.42	352586.07	339682.78
	(³ P) ² D	5/2	30	364819.62	359714.56	343709.55
	(³ P) ² P	1/2	29	363414.99	366274.62	346345.56
	(³ P) ² D	3/2	31	377428.37	372749.08	358168.09

^aLevel energy revised in present work.

Table 10

Comparison of present percentages (in bold type) for the $4s4p^6$ and $4s^24p^44d$ configurations with the percentage compositions of Singh et al [18] (in parentheses). Level values are in cm^{-1} . Index numbers are those used in [18] and [19]. Where there are no values in parentheses, no percentage was given by Singh et al [18].

Index	Singh label	J	E(obs) ^a	Percentage Composition			
3	$4s^2S$	1/2	191571	77(72)%	$4s^2S$	23(27)%	($1D$) ² S
4	(3P) ⁴ D	5/2	248940	88(90)%	(3P) ⁴ D	3%	(3P) ⁴ P 3% (3P) ⁴ F
5	(3P) ⁴ D	7/2	249323	91(93)%	(3P) ⁴ D	6%	(3P) ⁴ F 2% ($1D$) ² F
6	(3P) ⁴ D	3/2	250018	86(88)%	(3P) ⁴ D	4%	(3P) ⁴ P 3% ($1D$) ² D
7	(3P) ⁴ D	1/2	251819	85(89)%	(3P) ⁴ D	7%	($1D$) ² P 5% (3P) ² P
8	(3P) ⁴ F	9/2	261643	90(92)%	(3P) ⁴ F	10%	($1D$) ² G
9	(3P) ⁴ F	7/2	266145	66(75)%	(3P) ⁴ F	17%	(3P) ² F 13% ($1D$) ² G
10	($1D$) ² P	1/2	266279	44(44)%	($1D$) ² P	37(39)%	(3P) ² P 14% (3P) ⁴ D
12	(3P) ⁴ F	3/2	271296	48(74)%	(3P) ⁴ F	16%	(3P) ⁴ P 13% ($1S$) ² D
11	(3P) ⁴ F	5/2	271374	93(94)%	(3P) ⁴ F	3%	(3P) ⁴ D 2% ($1S$) ² D
13	(3P) ⁴ P	1/2	272091	91(91)%	(3P) ⁴ P	5%	(3P) ² P 3% ($1D$) ² P
14	(3P) ⁴ P	3/2	272834	38(50)%	(3P) ⁴ P	30%	(3P) ⁴ F 18(20)% ($1D$) ² P
15	($1D$) ² D	3/2	274666	36(40)%	($1D$) ² D	21(24)%	(3P) ² D 15% (3P) ⁴ F
16	(3P) ² F	7/2	276491	42(50)%	(3P) ² F	25(17)%	(3P) ⁴ F 20(20)% ($1D$) ² G
17	(3P) ⁴ P	5/2	278742	74(84)%	(3P) ⁴ P	9%	($1S$) ² D 7% (3P) ² D
18	(3P) ⁴ P	3/2	279457 ^b	40(24)%	(3P) ⁴ P	24(36)%	($1D$) ² P 22(22)% (3P) ² P
19	($1D$) ² D	5/2	283112	40(43)%	($1D$) ² D	21(23)%	(3P) ² D 18% (3P) ⁴ P
20	($1D$) ² G	7/2	285967	65(69)%	($1D$) ² G	24(21)%	(3P) ² F 10% ($1D$) ² F
21	($1D$) ² G	9/2	286412	90(92)%	($1D$) ² G	10%	(3P) ⁴ F
22	(3P) ² F	5/2	287142	65(64)%	(3P) ² F	21(19)%	($1D$) ² F 9% ($1D$) ² D
23	($1D$) ² F	5/2	299609	77(79)%	($1D$) ² F	12%	(3P) ² F 9% ($1D$) ² D
24	($1D$) ² F	7/2	303517	80(81)%	($1D$) ² F	16(16)%	(3P) ² F 2% ($1D$) ² G
25	($1S$) ² D	3/2	319336	63(66)%	($1S$) ² D	25(25)%	($1D$) ² D 5% ($1D$) ² P
26	($1S$) ² D	5/2	325577	73(74)%	($1S$) ² D	14%	($1D$) ² D 5% (3P) ² F

Index	Singh label	J	E(obs) ^a	Percentage Composition					
				(¹ D) ² S	(¹ D) ² S	(¹ D) ² S	4s ² S	(¹ D) ² P	(³ P) ² P
28	(¹ D) ² S	1/2	334695	69 (42)%	(¹ D) ² S	20 %		5 (21)%	4 (20)%
27	(³ P) ² P	3/2	339683	50 (52)%	(³ P) ² P	36 (40)%	(¹ D) ² P	7 %	(¹ D) ² D
30	(³ P) ² D	5/2	343710	64 (66)%	(³ P) ² D	21 (22)%	(¹ D) ² D	11 %	(¹ S) ² D
29	(³ P) ² P	1/2	346346	48 (32)%	(³ P) ² P	41 (27)%	(¹ D) ² P	7 (30)%	(¹ D) ² S
31	(³ P) ² D	3/2	358168	57 (60)%	(³ P) ² D	19 (17)%	(¹ S) ² D	14 (17)%	(¹ D) ² D

^aPresent value from table 3.

^bLabel for this level in present work is 4p⁴4d(¹D)²P_{3/2}.