



Article Core Effects on Transition Energies for $3d^k$ Configurations in Tungsten Ions

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Abstract: All energy levels of the $3d^k$, k = 1, 2, ..., 8, 9, configurations for tungsten ions, computed using the GRASP2K fully relativistic code based on the variational multiconfiguration Dirac–Hartree–Fock method, are reported. Included in the calculations are valence correlation where all 3s, 3p, 3d orbitals are considered to be valence orbitals, as well as core–valence and core–core effects from the 2s, 2p subshells. Results are compared with other recent theory and with levels obtained from the wavelengths of lines observed in the experimental spectra. It is shown that the core correlation effects considerably reduce the disagreement with levels linked directly to observed wavelengths, but may differ significantly from the NIST levels, where an unknown shift of the levels could not be determined from experimental wavelengths. For low values of k, levels were in good agreement with relativistic many-body perturbation levels, but for 2 < k < 8, the present results were in better agreement with observation.

Keywords: core correlation effects; energy levels; multiconfiguration Dirac-Hartree-Fock; tungsten ions

1. Introduction

Because of their importance for the ITER project [1], spectra of tungsten ions have recently received much attention over a wide range of wavelengths. Of special interest are the NIST EBIT experiments reported by Ralchenko et al. [2], who studied tungsten ions with the ground states 3d, $3d^2$, ..., $3d^8$, and $3d^9$. Detailed collisional-radiative modelling was undertaken to identify the measured spectral lines. For the modelling they relied on energy levels, radiative transition probabilities, and electron-impact collisional cross-sections obtained using the relativistic Flexible Atomic Code (FAC) [3]. They found that many of the strong lines arose from magnetic dipole (M1) transitions. These lines were located in a narrow range of wavelengths, mostly well isolated with line ratios that could infer plasma properties, and were sensitive to electron densities. All these features make the M1 lines useful for plasma diagnostics. The measured observed wavelengths for M1 transitions and the FAC energy levels were analyzed by Kramida [4] for spectra for these ions, and form the basis for the energy levels included in the Atomic Spectra Database (ASD) [5].

At the same time, highly charged ions are of special interest for theory in that both correlation and relativistic effects are interrelated, and additional quantum electrodynamic (QED) corrections are needed for accurate results. Quinet [6] reports an extensive summary of a large variety of theoretical energy levels and forbidden transitions for all levels of $3d^k$ ground configurations, and compared their energy levels with the NIST energies. Included among the various methods were results that he obtained using the GRASP code developed by Norrington [7]. Most of the correlation included in the calculation was valence correlation restricted to the n = 3 complex. More recently, Guo el al. [8] computed energy levels, wavelengths, and transition probabilities for the same configurations for a number of ions, including tungsten. The theoretical basis for their work was the relativistic many-body perturbation theory (RMBPT) as described in [9], but small corrections for finite nuclear size, nuclear recoil, vacuum polarization, and self-energy correction were also included using standard procedures such as those in GRASP2K [10]. All basis orbitals were determined from the same central field, and all three types of correlation—valence–valence (VV), core–valence (CV), and core–core (CC)—where the core consists of the the full 1*s*, 2*s*, 2*p* core were included . Statistically, their energy levels were in much better agreement with NIST values than those of Quinet [6].

The purpose of the present work was to evaluate the accuracy of energy levels obtained from variational multconfiguration Dirac–Hartree–Fock methods as implemented in the GRASP2K code [10]. Included are all three correlation types as in the RMBPT calculation—except for the $1s^2$ core, that will be assumed to be inactive.

2. Multiconfiguration Dirac–Hartree–Fock (MCDHF) and Configuration Interaction Methods

In the MCDHF method [11,12], as implemented in the GRASP2K program package [10], the wave function $\Psi(\gamma P J M_J)$ for a state labeled $\gamma P J M_J$, where *J* and M_J are the angular quantum numbers and *P* is the parity, is expanded in antisymmetrized and coupled configuration state functions (CSFs)

$$\Psi(\gamma P J M_J) = \sum_{j=1}^{M} c_j \Phi(\gamma_j P J M_J).$$
⁽¹⁾

The labels $\{\gamma_j\}$ denote other appropriate information about the CSFs, such as orbital occupancy and coupling of the subshells. The CSFs are built from products of one-electron orbitals, having the general form

$$\psi_{n\kappa,m}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa,m}(\theta,\varphi) \\ \iota Q_{n\kappa}(r)\chi_{-\kappa,m}(\theta,\varphi) \end{pmatrix},$$
(2)

where $\chi_{\pm\kappa,m}(\theta, \varphi)$ are two-component spin–orbit functions. The radial functions { $P_{n\kappa}(r)$, $Q_{n\kappa}(r)$ } are represented numerically on a grid.

Wave functions for a number of targeted states are determined simultaneously in the extended optimal level (EOL) scheme. Given initial estimates of the radial functions, the energies *E* and expansion coefficients $\mathbf{c} = (c_1, \dots, c_M)^t$ for the targeted states are obtained as solutions to the configuration interaction (CI) problem

$$\mathbf{Hc} = E\mathbf{c},\tag{3}$$

where **H** is the CI matrix of dimension $M \times M$ with elements

$$H_{ij} = \langle \Phi(\gamma_i P J M_J) | H | \Phi(\gamma_j P J M_J) \rangle.$$
(4)

Radial functions are solutions of systems of differential equations that define a stationary state of an energy functional for a wave function expansion.

Two types of expansions may be used. In the past, both usually were the same, but for large calculations, there are advantages to relaxing this restraint. The first is the expansion that determines the radial functions using the RMCDHF program of the GRASP2K package. For occupied orbitals, optimized radial functions can be obtained by applying the variational principal of an energy expression. However, when correlation orbitals are to be determined, the most effective orbitals are those that are in the same region of space as the occupied orbitals for a given type of correlation, as has been shown in partitioned configuration interaction (PCFI) studies [13]. In this work, we consider two regions: the 3s, 3p, 3d region for valence–valence (VV) correlation and the 2s, 2p region for core–valence (CV) and core–core (CC) correlations.

The second is an expansion for the relativistic configuration interaction (RCI) program that determines the wavefunction and its associated energy for a given Hamiltonian and based on a given orbital basis. In the present work, the Hamiltonian for RCI was the Dirac–Coulomb Hamiltonian (DC) plus the transverse photon interaction (DCB), the vacuum polarization effects as accounted for by the Uehling potential, and electron self-energies as calculated with the screened hydrogenic formula [12,14], namely the DCBQ Hamiltonian. The RCI program is relatively simple to parallelize efficiently [15,16] using message passing. As a result, much larger expansions are possible for RCI calculations than RMCDHF ones that build the orbital basis. Present calculations were done with forty-eight (48) processors for the larger cases.

The computational procedure was essentially the same for all ions. The first step was to perform Dirac-Hartree-Fock (DHF) calculations (in the EOL approximation) for all states associated with the $3s^23p^63d^k$ configuration. This calculation determined the 1s, 2s, 2p orbitals for all subsequent calculations. Then, sequentially, orbital sets of increasing size, with maximum principal quantum numbers n = 3, 4, 5, were determined from expansions that defined valence-valence correlation expansions. The latter were obtained from single- and double-excitations from the valence shells to those of the orbital set. Since the 3d shell is unfilled, excitations such as $3s^2 \rightarrow 3d^2$ are allowed and increase the generalized occupation number for the 3d orbitals but decrease those of 3s. Variational methods determined the new orbitals introduced at each stage using the Dirac-Coulomb Hamiltonian. The n = 6 orbitals were targeted for core correlation effects. They were obtained from calculations that included CV correlation from the n = 2 shell where one orbital from the active core (either 2s or 2p) and one 3s, 3p, or 3d orbital were excited, as well as CC, where two n = 2 orbitals were excited. At the same time, excitations from 3s, 3p subshells were limited to single excitations for 3s or 3p, thereby contracting the n = 6 orbitals to overlap more strongly with the n = 2 orbitals and reducing the size of the expansions. For the configurations $3d^k$, k = 3, 4, 5, 6, 7, the expansions were still exceedingly large and additional restrictions on interactions were imposed that define the energy functional. First, what might be considered a zero-order approximation was obtained that consisted of the CSFs of the n = 5 VV expansion that accounted for 99.9 percent of the normalized expansion. All other terms of the n = 6 expansions were treated as first-order corrections. In deriving the energy expression that determines the radial factors of the n = 6 orbitals, it was assumed that the interaction between CSFs of the first-order corrections could be neglected. This procedure optimizes the interaction of the n = 6 orbitals with the zero-order wave function, and has the effect of contracting the core-valence orbitals.

Each of these four orbital sets were then used in relativistic configuration interaction (RCI) calculations that included VV, CV, and CC correlation effects (excluding the 1*s* shell) for the three Hamiltonians—DC, DCB, and DCBQ. Again, for the cases where k = 3, 4, 5, 6, 7, the RCI calculations were performed under the assumption that interactions between CSF of the first-order correction could be ignored.

J	M	т	J	M	т
3d			3d ⁹		
3/2	103 104	-	3/2	152 230	-
5/2	130 021	-	5/2	193 718	-
$3d^2$			3d ⁸		
0	109 376	-	0	138 241	-
1	306 873	-	1	388 664	-
2	453 546	-	2	576 194	-
3	526 871	-	3	672 708	-
4	529 065	-	4	679 881	-
$3d^3$			$3d^{7}$		
1/2	508 854	514	1/2	584 675	734
3/2	934 941	1056	3/2	$1\ 075\ 476$	1564
5/2	1 217 067	1 062	5/2	1 402 693	1 563
7/2	1 328 694	668	7/2	1 535 467	1 0 2 0
9/2	1 281 840	737	9/2	$1\ 486\ 446$	$1\ 055$
11/2	2216460	277	11/2	1 300 160	353
$3d^4$			3d ⁶		
0	433 540	925	0	462 613	1 113
1	1 228 917	$1\ 070$	1	1 311 786	1 244
2	$1\ 840\ 515$	1688	2	1 965 798	2 071
3	2 187 525	1 375	3	2 338 660	1 738
4	2 261 243	1 624	4	2 420 366	1 921
5	2 095 354	632	5	2 246 438	761
6	1 771 535	572	6	1 902 774	659
$3d^{5}$					
1/2	1 022 700	1 119			
3/2	$1\ 888\ 910$	1688			
5/2	2 480 422	2 352			
7/2	2 741 429	1 857			
9/2	2 687 207	1 306			
11/2	2 387 571	910			
13/2	1 943 915	329			

Table 1. Table showing the size (*M*) of the n = 6 relativistic configuration interaction (RCI) expansions and the size of the zero-order space (*m*) for the different tungsten ions.

Table 1 summarizes the size of various expansions for the different $3d^k$ configurations, whereas Table 2 shows how the mean radii of the n = 6 orbitals are contracted relative to the valence correlation orbitals. Note that the size increases rapidly as the number of electrons (or holes) increases from one to five, as well as the number of *J* values and levels. The number of CSFs defining 99.9% of the wave function composition is relatively small. Increasing this percentage to 99.99% would include some higher order corrections. As for mean radii, it should be noted the the 3*d* orbitals (in non-relativistic notation) have a mean radius closer to the core than either 3*s* or 3*p*. Listed in Table 2 are typical values for the $3d^5$ configuration. The mean radii are also depicted graphically in Figure 1. Correlation increases the generalized orbital occupation number of the 3*d* orbitals, but decreases those of all other occupied orbitals. The n = 4 and n = 5 orbitals have mean radii similar to those of the valence orbitals, whereas the n = 6 orbitals that are used to represent CC and CV correlation have mean radii either similar to n = 2 orbitals or between n = 2 and n = 3, as in CV correlation.

nl	$\langle nl r nl \rangle$	w
1s	1.83433D-02	2.00000
2s	7.64525D-02	1.99992
$2p_{-}$	6.33222D-02	1.99986
2p	7.10859D-02	3.99969
3s	1.91692D-01	1.99940
$3p_{-}$	1.81324D-01	1.99853
3p	1.93743D-01	3.99577
$3d_{-}$	1.67488D-01	2.00137
3 <i>d</i>	1.71346D-01	3.00266
4s	2.04509D-01	1.24D-04
$4p_{-}$	1.89988D-01	1.45D-04
4p	2.01490D-01	2.94D-04
$4d_{-}$	1.71036D-01	1.73D-04
4d	1.70979D-01	2.82D-04
$4f_{-}$	1.94058D-01	5.94D-04
4f	1.97398D-01	8.24D-04
5s	2.03090D-01	1.93D-05
$5p_{-}$	1.95387D-01	2.23D-05
5p	1.97508D-01	4.08D-05
$5d_{-}$	2.12303D-01	2.88D-05
5d	2.17420D-01	4.47D-05
$5f_{-}$	1.86560D-01	1.30D-05
5f	1.85984D-01	2.01D-05
$5g_{-}$	1.97882D-01	3.38D-05
5g	2.00859D-01	5.11D-05
6 <i>s</i>	1.31230D-01	6.77D-06
$6p_{-}$	1.19574D-01	8.04D-06
6 <i>p</i>	1.20726D-01	1.40D-05
$6d_{-}$	1.18546D-01	1.71D-05
6d	1.24725D-01	2.58D-05
$6f_{-}$	8.84520D-02	7.35D-06
6 <i>f</i>	9.29611D-02	1.10D-05
6g_	7.72823D-02	2.26D-06
6g	7.88248D-02	3.31D-06
$6h_{-}$	1.62256D-01	2.42D-06
6h	8.04121D-02	7.65D-07

Table 2. Mean radii in a.u. of orbitals for the $3d^5$ configuration and their generalized occupation number *w*.

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Figure 1. Plot of the mean radii of orbitals of the $3d^5$ configuration in the order listed in Table 2.

3. Results and Their Comparison

Table 3 reports some of the results for all levels of the $3d^k$ configurations of tungsten ions from RCI calculations for the DCBQ Hamiltonian. The classification of energy levels are presented in the LSJ- and *jj*-couplings. A set of three quantum numbers L, S, and seniority ν allows a one-to-one classification of $3d^k$ (k = 3, 4, 5, 6, 7) energy levels in LSJ-coupling. These quantum numbers are presented in Table 3 as ${}^{(2S+1)}L^{\nu}$. The n = 5 results include only VV correlation, whereas n = 6 include all three correlation effects. The next column is the energy levels as reported by NIST [5]. Included here are the different types of results. Energies with no square brackets are directly related to observed wavelengths—often these are in the lower portion of the spectrum. Then, there are levels that may be linked to an observed wavelength but the shift of the energy levels relative to the ground state is not known from experiment. These levels include a +x or +y in the table. Thus, the difference between two levels with the same +x is known accurately, but not the levels themselves. Taking these factors into account, it is clear that the inclusion of core effects has reduced the discrepancy with NIST values by about a factor of 1/2. In the next column, the values found by Quinet [6] are generally like the VV results. From a general theoretical point of view, the the RMBPT results of Guo et al. [8] should be the most accurate. In the case of $3d^2$, RMBPT results have also been reported by Safronova and Safronova [17], and are reported in the last column. These results are not as accurate as those of Guo et al. In these tables, all energies are reported in the units of 1000 cm^{-1} .

Table 3. Energy level results for 3d, $3d^2$, ..., $3d^8$, $3d^9$ ground configuration of tungsten ions. Shown is a unique label in *LSJ*- and *jj*-notation, the *J* value, the present n = 5 result for valence–valence (VV) correlation, and n = 6 result for all three types of correlation, the Atomic Spectra Database (ASD) value [5], the Quinet value [6], the Guo et al. RMBPT_g value [8], and the Safronova & Safronova RMBPT_s value [17]. All energy levels are reported in 1000 cm⁻¹.

	Label		т	Presen	t Work		CDACD	DMDDT	DMPDT
LSJ-	jj-Co	uplings	J	n = 5	n = 6	ASD	GKASI	KWIDF 1g	KIVIDI I S
W ⁵⁵⁺ (K	-like)								
3d ² D	3 <i>d</i> _	(3/2,0)	3/2	0.00	0.00	0.00	0.00	0.00	
3d ² D	$3d_+$	(0,5/2)	5/2	625.23	626.17	626.49	624.7	626.56	
W ⁵⁴⁺ (C	a-like)								
$3d^{2} {}^{3}F$	$3d_{-}^{2}$	(2,0)	2	0.00	0.00	0.00	0.00	0.00	0.00
$3d^{2} {}^{3}P$	$3d_{-}^{2}$	(0,0)	0	186.42	186.23	[188]	186.9	184.86	187.11
$3d^{2} {}^{3}F$	$3d_{-}3d_{+}$	(3/2,5/2)	3	584.05	584.75	585.48	583.5	585.80	582.85
$3d^{2} {}^{3}P$	$3d_{-}3d_{+}$	(3/2,5/2)	2	667.45	667.96	668.49	667.6	668.00	666.21
$3d^{2} {}^{3}P$	$3d_{-}3d_{+}$	(3/2,5/2)	1	706.35	706.75	709.46+x	707.1	706.78	705.41
$3d^{2} {}^{1}G$	$3d_{-}3d_{+}$	(3/2,5/2)	4	695.68	696.10	[697]	697.1	696.74	693.81
$3d^{2} {}^{3}F$	$3d_{+}^{2}$	(0,4)	4	1234.31	1235.57	[1234]	1234.1	1237.00	1231.64
$3d^{2} {}^{3}P$	$3d_{+}^{2}$	(0,2)	2	1298.91	1300.18	[1299]	1298.6	1300.28	1296.73
$3d^2 {}^1S$	$3d_{+}^{2}$	(0,0)	0	1492.04	1493.71	[1493]	1491.0	1491.18	1491.54
W ⁵³⁺ (So	z-like)								
$3d^{3} {}^{4}F^{3}$	$3d_{-}^{3}$	(3/2,0)	3/2	0.00	0.00	0.00	0.00	0.00	
$3d^{3} {}^{4}F^{3}$	$3d_{-}^{2}3d_{+}$	(2,5/2)	5/2	528.39	529.07	530.03	528.2	530.51	
$3d^{3} {}^{4}P^{3}$	$3d_{-}^{2}3d_{+}$	(2,5/2)	3/2	579.43	579.99	580.86	579.9	580.86	
$3d^{3} {}^{2}G^{3}$	$3d_{-}^{2}3d_{+}$	(2,5/2)	7/2	610.41	610.86	[610]	611.7	611.86	
$3d^{3} {}^{4}P^{3}$	$3d_{-}^{2}3d_{+}$	(2,5/2)	1/2	622.72	623.22	623.95	623.6	623.53	
$3d^{3} {}^{2}H^{3}$	$3d_{-}^{2}3d_{+}$	(2,5/2)	9/2	609.94	610.32	[610]+x	612.0	611.62	
$3d^{3} {}^{2}D^{1}$	$3d_{-}^{2}3d_{+}$	(0,5/2)	5/2	811.84	812.07	812.22	814.2	811.77	
$3d^{3} {}^{4}F^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,4)	7/2	1127.31	1128.60	[1126]	1127.1	1130.58	
$3d^{3} {}^{4}F^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,4)	9/2	1164.81	1165.99	[1164]	1165.7	1168.15	
$3d^{3} {}^{4}P^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,2)	3/2	1206.41	1207.73	[1206]	1206.2	1208.34	

	Label		T	Presen	t Work	450	CDASD	DMBDT	DMPDT		
LSJ-	<i>jj-</i> Co	uplings	J	n = 5	n = 6	ASD	GRASI	KWIDI 1g	KWIDF 1 _S		
$3d^{3} {}^{2}P^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,2)	1/2	1230.34	1231.58	[1230]	1230.5	1232.08			
$3d^{3} {}^{2}D^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,4)	5/2	1243.67	1244.61	[1244]	1245.0	1245.39			
$3d^{3} {}^{2}H^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,4)	11/2	1242.38	1243.30	1243.51+x	1245.2	1245.42			
$3d^{3} {}^{2}F^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,2)	5/2	1314.58	1315.54	[1315]	1316.4	1315.84			
$3d^{3} {}^{2}F^{3}$	$3d_{-}3d_{+}^{2}$	(3/2,2)	7/2	1318.68	1319.55	[1320]	1321.5	1320.10			
$3d^{3} {}^{2}D^{1}$	$3d_{-}3d_{+}^{2}$	(3/2,0)	3/2	1479.96	1481.26	[1482]	1481.3	1479.89			
$3d^{3} {}^{2}G^{3}$	$3d^3_{\perp}$	(0,9/2)	9/2	1762.93	1764.86		1762.9	1767.02			
$3d^{3} {}^{2}P^{3}$	$3d_{\perp}^{3}$	(0,3/2)	3/2	1876.44	1878.32		1877.0	1878.54			
$3d^{3} {}^{2}D^{1}$	$3d_{+}^{3}$	(0,5/2)	5/2	1958.00	1960.12		1957.9	1959.56			
W ⁵²⁺ (Ti	-like)										
$3d^{4} {}^{3}P^{2}$	$3d^4$	(0,0)	0	0.00	0.00	0.00	0.00	0.00			
$3d^{4} {}^{5}D^{4}$	$3d^{3} 3d_{+}$	(3/2.5/2)	1	515.87	516.51	517.63	516.0	518.08			
$3d^{4} {}^{3}H^{4}$	$3d^3 3d_{\perp}$	(3/2.5/2)	4	613.24	613.54	[613]+v	615.6	614.79			
$3d^{4} {}^{5}D^{4}$	$3d^3 3d_+$	(3/2.5/2)	2	637.98	638.39	[638]+x	639.9	639.34			
$3d^{4} {}^{3}F^{2}$	$3d^3 3d_{\perp}$	(3/2.5/2)	3	665.84	666.09	665.5621+x	668.6	667.04			
$3d^{4} {}^{5}D^{4}$	$3d^2 3d^2$	(2,2)	0	1101.86	1103.18	[1100]	1101.6	1104.66			
$3d^{4} {}^{5}D^{4}$	$3d^2 3d^2$	(2.4)	2	1106.82	1107.98	1109.69	1107.6	1110.02			
$3d^{4} {}^{3}H^{4}$	$3d^2 3d^2$	(2,4)	4	1125.54	1126.59	1127.27+v	1127.3	1129.11			
$3d^{4} {}^{5}D^{4}$	$3d^2 3d^2$	(2.4)	3	1142.02	1143.02	[1141]	1144.0	1145.19			
$3d^{4} {}^{3}H^{4}$	$3d^2 3d^2$	(2.4)	5	1172.24	1173.06	1173.35 + v	1175.7	1175.60			
$3d^{4} {}^{3}D^{4}$	$3d^2 3d^2$	(2,1)	1	1213.52	1214 54	[1213]	1215.4	1215.64			
$3d^{4} {}^{1}I^{4}$	$3d^2 3d^2$	(2,2)	6	1195.60	1196.31	[1195]	1200.00	1199.02			
$3d^{4} {}^{3}F^{4}$	$3d^2 3d^2$	(2,1)	3	1239.13	1239.92	[1240]	1242.5	1240.99			
$3d^{4} {}^{3}G^{4}$	$3d^2 3d^2$	(2,2)	4	1242 41	1243 17	[1243]	12457	1244 47			
$3d^{4} {}^{3}F^{4}$	$3d^2 3d^2$	(2,2)	2	1257 75	1258.62	[1258]	1260.6	1259.43			
$3d^{4} {}^{3}F^{2}$	$3d^2 3d^2$	(2,2)	2	1359.28	1360.02	[1361]	1361.1	1360 35			
$3d^{4} {}^{3}F^{2}$	$3d^2 3d^2$	(0.4)	4	1403.66	1404 22	1403.95 + x	1408.6	1405 11			
$3d^{4} {}^{1}D^{2}$	$3d^2 3d^2$	(0,1)	2	1505.68	1506.35	[1509]	1510.3	1505.82			
$3d^{4} 3p^{4}$	$3d^2 3d^2$	(0,2)	0	1633.13	1634 15	[1637]	1636.5	1632 74			
3d4 5D4	$3d_{3d}$	(0,0) (3/2.9/2)	4	1714.26	1715 10	[1057]	1715.3	1718 50			
3d4 3E4	$3d 3d^3$	(3/2, 9/2)	т 2	1725.24	1713.10		1715.5	1710.00			
3d4 3D4	$3d 3d^3$	(3/2, 3/2)	1	1766 70	1768 58		1723.7	1729.13			
$3d4 \ 3c4$	$3d 3d^3$	(3/2,3/2)	5	1773 76	1700.00		1707.1	1707.70			
314 3 H4	$3d 3d^3$	(3/2, 9/2)	6	1778 76	1780.20		1782 /	1783.28			
3d4 3E4	$3d 3d^3$	(3/2, 3/2)	2	18/1 18	1842.08		1842.4	1843.90			
3d4 3D4	$3d 3d^3$	(3/2,3/2)	2	1857 70	1859 24		1860.2	1860.18			
3d4 1 54	$3d 3d^3$	(3/2,3/2)	0	1022.88	1037.24		1925.8	1923 37			
314 3 D2	$3d 3d^3$	(3/2,3/2)	1	1922.00	1924.00		1923.0	1925.57			
3u = 1 $2d = 3r^2$	$3u_{-}3u_{+}$	(3/2,3/2)	1	1070.06	1905.44		1907.2	1905.44			
3u F $2d^{4} 1C^{2}$	$3u_{-}3u_{+}$	(3/2,3/2)	3	1979.90	1961.50		1903.0	1901.91			
3 <i>μ</i> G	$3u_{-}3u_{+}^{-}$	(3/2,3/2)	4	1965.00	1900.37		1900.7	2010.68			
5и D 2 44 3 г2	$3u_{-}3u_{+}^{-}$	(3/2,3/2)	ے 1	2010.03	2020.04		2022.0	2019.00			
3d4 1 D2	$3u_+$ $3d^4$	$(0, \pm)$	4 ว	23/0.23	23/0.00		23/0.1	2300.31			
$3d^{4} {}^{3} p^{2}$	$3d^4$	(0, 2) (0, 0)	∠ 0	2400.31 2662 74	2403.00 2665 52		2401.4 2663 5	2403.30 2663.60			
W^{51+} (V	like)	(0,0)	0	2002.7 म	2000.02		2005.5	2005.00			
245403	2.14.2.1	$(0 \in (2))$	E (0	0.00	0.00	0.00	0.00	0.00			
3a ⁵ 7P ⁵	$3a_{\pm}^{\pm}3a_{\pm}$	(0, 5/2)	5/2 E/2	0.00	0.00	0.00	0.00	0.00			
$3u^{\circ} {}^{\circ} S^{\circ}$	$3u^{2}_{-}3a^{2}_{+}$	(3/2,4)	5/2	409./1	4/0./5	/1.63	469.1	4/2.03			
3a° ±G°	3a_3a_+	(3/2,4)	7/2	564.98	565.80	66.25	566.2	566.41			

Table 3. Cont.

	Label		_	Presen	t Work				
LSJ-	jj-Co	uplings	J	n = 5	n = 6	ASD	GRASP	RMBPT _g	RMB
$3d^{5} {}^{4}D^{5}$	$3d^3 3d^2$	(3/2.2)	3/2	579.61	580.50	80.89	579.8	580.44	
$3d^{5} {}^{2}H^{3}$	$3d^3 3d^2$	(3/2.4)	11/2	576.03	576.78	[577]+x	578.5	577.80	
$3d^{5} {}^{2}G^{5}$	$3d^3 3d^2$	(3/2.4)	9/2	620.92	621.61	[623]	623.7	622.20	
$3d^{5} {}^{4}D^{5}$	$3d^3 3d^2$	(3/2.2)	5/2	650.71	651.45	[652]	652.8	651.27	
$3d^{5} 4p^{3}$	$3d^3 3d^2$	(3/22)	1/2	679.60	680.38	[681]	680.8	679.83	
$3d^{5} {}^{2}F^{5}$	$3d^3 3d^2$	(3/2,2)	7/2	687 73	688.28	88 18	690.9	687.90	
$3d^{5} 2D^{1}$	$3d^3 3d^2$	(3/2,2)	3/2	873.99	824.95	[827]	825.5	823.60	
3d5 6c5	$3d^2 3d^3$	(3/2,0) (2.9/2)	5/2	1025.98	1027.97	[1015]	1024.9	1029.10	
3d ⁵ 4D ⁵	$3d^2 3d^3$	(2,9/2)	7/2	1025.90	1027.57	[1013]	1024.7	1029.11	
$3d^5 4C^5$	$3d^2 3d^3$	(2,9/2)	11/2	1100.04	1102 51	1103/13	1103.0	1079.09	
$3d^5 4C^5$	$3d^2 3d^3$	(2, 9/2)	0/2	1116.08	1118 70	[1118]	1118.8	11104.04	
245405	$3u_{-}3u_{+}$	(2,3/2)	9/2 1/2	1110.90	1110.70	[1110]	1110.0	1119.70	
2 45 4 D ²	$3u_{-}^{2}3u_{+}^{2}$	(2,3/2)	1/2	1100.00	1107.40		1100.0	1137.33	
30° - P°	$3u_{-}^{2}3u_{+}^{2}$	(2,3/2)	3/2	1104.73	1100.79	[1140]	1103.0	1100.04	
$3u^2 - 1^2$ $2u^5 2 r^5$	$3u_{-}^{2}3u_{+}^{2}$	(2,9/2)	13/2	1142.15	1145.78	[1143]	1145.6	1145.272	
$3a^{\circ} = F^{\circ}$	$3a_{-}^{-}3a_{+}^{0}$	(2,3/2)	5/2	11/4.89	11/6.61		11/6.3	11/6.63	
$3a^{\circ} = H^{\circ}$	$3a_{-}^{2}3a_{+}^{3}$	(2,5/2)	9/2	1217.34	1219.21		1218.4	1219.39	
$3d^{5} = G^{5}$	$3d_{-}^{2}3d_{+}^{3}$	(2,3/2)	7/2	1237.88	1239.44		1240.9	1239.13	
$3d^{5} = F^{5}$	$3d_{-}^{2}3d_{+}^{3}$	(2,5/2)	5/2	1254.59	1256.46		1255.8	1256.02	
$3d^{3} + D^{3}$	$3d_{-}^{2}3d_{+}^{3}$	(2,3/2)	3/2	1259.49	1260.94		1262.1	1259.77	
$3d^{5} = P^{5}$	$3d_{-}^{2}3d_{+}^{3}$	(2,5/2)	1/2	1308.19	1309.93		1309.8	1308.63	
$3d^{5} = G^{5}$	$3d_{-}^{2}3d_{+}^{3}$	(2,5/2)	7/2	1307.82	1309.62		1309.9	1308.84	
$3d^5 {}^2G^3$	$3d_{-}^{2}3d_{+}^{3}$	(0,9/2)	9/2	1379.66	1381.18		1383.8	1380.57	
$3d^{5} {}^{2}P^{3}$	$3d_{-}^{2}3d_{+}^{3}$	(0,3/2)	3/2	1504.94	1506.22		1510.4	1504.14	
$3d^{5} {}^{2}D^{1}$	$3d_{-}^{2}3d_{+}^{3}$	(0,5/2)	5/2	1533.17	1534.71		1537.4	1532.74	
$3d^5 \ ^4P^3$	$3d_{-}3d_{+}^{4}$	(3/2,4)	5/2	1660.92	1663.98		1658.7	1664.07	
$3d^{5} {}^{4}F^{3}$	$3d_{-}3d_{+}^{4}$	(3/2,4)	7/2	1733.68	1736.62		1733.1	1736.60	
$3d^{5} {}^{4}D^{5}$	$3d_{-}3d_{+}^{4}$	(3/2,2)	3/2	1759.25	1762.30		1758.1	1761.85	
$3d^{5} {}^{2}H^{3}$	$3d_{-}3d_{+}^{4}$	(3/2,4)	11/2	1746.45	1749.34		1747.2	1749.91	
$3d^{5} {}^{2}G^{5}$	$3d_{-}3d_{+}^{4}$	(3/2,4)	9/2	1806.21	1808.95		1807.7	1808.86	
$3d^{5} {}^{2}D^{3}$	$3d_{-}3d_{+}^{4}$	(3/2,2)	5/2	1843.82	1846.49		1844.6	1845.21	
$3d^{5} {}^{2}G^{3}$	$3d_{-}3d_{+}^{4}$	(3/2,2)	7/2	1871.70	1874.38		1874.1	1873.74	
$3d^{5} {}^{2}P^{3}$	$3d_{-}3d_{+}^{4}$	(3/2,2)	1/2	1933.91	1936.39		1937.0	1934.46	
$3d^{5} {}^{2}D^{1}$	$3d_{-}3d_{+}^{4}$	(3/2,0)	3/2	2063.04	2065.78		2065.5	2062.96	
$3d^{5} {}^{2}D^{1}$	$3d_{+}^{5}$	(0,5/2)	5/2	2362.48	2366.70		2359.4	2365.33	
W ⁵⁰⁺ (C	r-like)								
3d ⁶ ⁵ D ⁴	$3d_{-}^{4}3d_{+}^{2}$	(0,4)	4	0.00	0.00	0.00	0.00	0.00	
$3d^{6} {}^{3}D^{4}$	$3d_{-}^{4}3d_{+}^{2}$	(0,2)	2	62.74	62.71	62.38	62.6	61.56	
$3d^{6} {}^{3}P^{2}$	$3d_{-}^{4}3d_{+}^{2}$	(0,0)	0	207.31	207.66	[208]+x	205.9	205.74	
$3d^{6} {}^{5}D^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,9/2)	3	506.28	507.09	508.03	505.2	507.80	
$3d^{6} {}^{5}D^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,9/2)	4	518.36	519.02	519.78	518.0	519.83	
$3d^{6} {}^{5}D^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,3/2)	1	545.62	546.54	[545]	543.8	546.53	
$3d^{6} \ {}^{3}G^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,9/2)	5	582.70	583.09	583.67	584.2	583.74	
$3d^{6} {}^{3}H^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,9/2)	6	582.40	582.70	[583]	584.3	583.61	
$3d^{6} {}^{3}F^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,3/2)	2	637.99	638.51	[639]	638.1	637.59	
$3d^{6} \ ^{3}D^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,3/2)	3	649.76	650.29	650.91	650.6	649.82	
$3d^{6} {}^{3}P^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,3/2)	0	725.01	725.35	[729]	727.9	723.98	
$3d^{6} {}^{3}P^{2}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,5/2)	1	767.07	767.54	768.98+x	769.3	766.38	
$3d^{6} {}^{3}D^{4}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,5/2)	2	766.25	766.84	766.95	767.6	765.69	
$3d^{6} {}^{1}G^{2}$	$3d^{3} 3d^{3}$	(3/2.5/2)	4	760.65	761.12	761.21	762.5	760.28	
-	+	(, ,-,-,)							

Table 3. Cont.

	Label			Presen	t Work				
LSJ-	jj-Co	uplings	J	n = 5	n = 6	ASD	GRASP	RMBPT _g	RMBPT _s
$3d^{6} {}^{3}F^{2}$	$3d_{-}^{3}3d_{+}^{3}$	(3/2,5/2)	3	782.18	782.54	782.53	785.0	781.26	
$3d^{6} {}^{5}D^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,4)	2	1058.57	1060.19		1055.6	1060.64	
$3d^{6} {}^{5}D^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,2)	0	1083.07	1084.88		1079.6	1085.16	
$3d^{6} {}^{3}H^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,4)	4	1108.16	1109.55		1106.9	1110.13	
$3d^{6} {}^{5}D^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,4)	3	1135.23	1136.57		1134.6	1136.84	
$3d^{6} {}^{3}H^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,4)	5	1142.11	1143.32		1142.4	1144.11	
$3d^{6\ 1}I^4$	$3d_{-}^{2}3d_{+}^{4}$	(2,4)	6	1169.18	1170.23		1170.5	1171.16	
$3d^{6} {}^{3}F^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,2)	3	1196.79	1198.08		1197.0	1198.01	
$3d^{6} {}^{3}D^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,2)	1	1217.26	1218.50		1217.8	1217.79	
$3d^{6} {}^{1}G^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,2)	4	1232.82	1233.95		1234.1	1233.73	
$3d^{6} {}^{3}F^{4}$	$3d_{-}^{2}3d_{+}^{4}$	(2,2)	2	1243.66	1244.79		1244.0	1243.75	
$3d^{6} {}^{3}F^{2}$	$3d_{-}^{2}3d_{+}^{4}$	(2,0)	2	1336.95	1338.38		1336.9	1336.97	
$3d^{6} {}^{3}F^{2}$	$3d_{-}^{2}3d_{+}^{4}$	(0,4)	4	1374.79	1375.77		1376.9	1375.03	
$3d^{6} \ ^{1}D^{2}$	$3d_{-}^{2}3d_{+}^{4}$	(0,2)	2	1518.97	1519.86		1523.2	1517.58	
$3d^{6} {}^{1}S^{0}$	$3d_{-}^{2}3d_{+}^{4}$	(0,0)	0	1660.58	1661.58		1664.9	1658.28	
$3d^{6} {}^{3}P^{2}$	$3d_{-}3d_{+}^{5}$	(3/2,5/2)	1	1663.26	1665.83		1657.7	1665.57	
$3d^{6} {}^{1}G^{2}$	$3d_{-}3d_{+}^{5}$	(3/2,5/2)	4	1764.33	1766.52		1762.0	1766.29	
$3d^{6} {}^{3}P^{2}$	$3d_{-}3d_{+}^{5}$	(3/2,5/2)	2	1813.76	1815.87		1811.7	1814.75	
$3d^{6} {}^{3}F^{2}$	$3d_{-}3d_{-}^{+}$	(3/2,5/2)	3	1831.23	1833.30		1830.3	1832.64	
$3d^{6} {}^{3}P^{2}$	$3d_{+}^{6}$	(0,0)	0	2321.86	2325.36		2314.1	2323.82	
W ⁴⁹⁺ (M	In-like)								
$3d^{7} {}^{4}F^{3}$	$3d_{-}^{4}3d_{+}^{3}$	(0,9/2)	9/2	0.00	0.00	0.00	0.00	0.00	
$3d^{7} {}^{2}P^{3}$	$3d_{-}^{4}3d_{+}^{3}$	(0,3/2)	3/2	101.71	101.64	[103]+x	102.1	100.13	
$3d^{7} {}^{2}D^{1}$	$3d_{-}^{4}3d_{+}^{3}$	(0,5/2)	5/2	158.95	159.10	158.75	158.7	157.62	
$3d^{7} {}^{4}F^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,4)	7/2	527.98	528.88	529.66	526.1	529.08	
$3d^{7} {}^{4}F^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,4)	9/2	583.50	584.16	584.59	583.1	584.18	
$3d^{7} {}^{4}P^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,2)	3/2	607.96	608.87	[608]	606.6	608.30	
$3d^{7} {}^{4}P^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,4)	5/2	624.97	625.72	628.02+x	624.9	625.41	
$3d^{7} {}^{4}P^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,2)	1/2	635.89	636.62	638.62+x	635.1	635.45	
$3d^{7} {}^{2}H^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,4)	11/2	650.16	650.58	650.70	651.8	650.55	
$3d^{7} {}^{2}F^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,2)	7/2	705.20	705.71	705.92	706.4	704.86	
$3d^{7} {}^{2}F^{3}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,2)	5/2	742.86	743.30	[747]	745.4	742.07	
$3d^{7} {}^{2}D^{1}$	$3d_{-}^{3}3d_{+}^{4}$	(3/2,0)	3/2	888.41	889.03	[893]	890.8	886.67	
$3d^{7} {}^{4}F^{3}$	$3d^{2}_{-}3d^{5}_{-}$	(2,5/2)	5/2	1115.46	1117.19		1112.0	1116.93	
$3d^{7} {}^{4}P^{3}$	$3d_{-}^{2}3d_{+}^{5}$	(2,5/2)	3/2	1147.62	1149.25		1145.1	1148.65	
$3d^{7} {}^{2}P^{3}$	$3d^{2}_{-}3d^{5}_{-}$	(2,5/2)	1/2	1192.13	1193.65		1189.9	1192.53	
$3d^{7} {}^{2}H^{3}$	$3d^{2}_{-}3d^{5}_{-}$	(2,5/2)	9/2	1185.68	1187.07		1184.9	1186.89	
$3d^{7} {}^{2}F^{3}$	$3d^{2}_{-}3d^{5}_{-}$	(2,5/2)	7/2	1210.79	1212.16		1210.3	1211.44	
$3d^{7} {}^{2}D^{1}$	$3d^2_{-}3d^5_{+}$	(0,5/2)	5/2	1410.07	1411.30		1411.0	1409.49	
$3d^{7} {}^{2}D^{1}$	$3d_{-}3d_{+}^{6}$	(3/2,0)	3/2	1751.87	1754.44		1746.4	1753.15	
W ⁴⁸⁺ (Fe	e-like)								
3d ⁸ ³ F	$3d_{-}^{4}3d_{+}^{4}$	(0,4)	4	0.00	0.00	0.00	0.00	0.00	
$3d^{8} {}^{1}D$	$3d_{-}^{4}3d_{+}^{4}$	(0,2)	2	72.15	72.12	[73.4]+x	72.8	71.26	
3d ^{8 3} P	$3d_{-}^{4}3d_{+}^{4}$	(0,0)	0	229.94	230.10	[233]	230.7	228.17	
3d ^{8 3} F	$3d_{-}^{3}3d_{+}^{5}$	(3/2,5/2)	3	525.18	526.07	526.65	523.2	526.13	
3d ^{8 3} P	$3d_{-}^{3}3d_{-}^{5}$	(3/2,5/2)	2	600.38	601.15	603.12+x	599.7	600.69	
3d ^{8 3} P	$3d_{-}^{3}3d_{+}^{5}$	(3/2,5/2)	1	642.01	642.71	644.76+x	642.7	642.14	
$3d^{8} {}^1G$	$3d_{-}^{3}3d_{+}^{5}$	(3/2,5/2)	4	643.89	644.43	644.70	645.0	644.03	

Table 3. Cont.

Label LSI- <i>ii</i> -Couplings		J	Presen	t Work	ASD	GRASP	RMBPT _g	RMBPT _s	
L5J-	<i>jj-</i> C0	jj-Couplings		n = 5	$n \equiv 0$			-	
3d ⁸ ³ F	$3d_{-}^{2}3d_{+}^{6}$	(2,2)	2	1106.91	1108.59	[1106]	1103.6	1108.17	
3d ⁸ ¹ S	$3d_{-}^{2}3d_{+}^{6}$	(0,0)	0	1304.16	1305.75	[1306]	1301.7	1304.07	
W^{47+} (C	Co-like)								
3d ⁹ ² D	$3d_{-}^{4}3d_{+}^{5}$	(0,5/2)	5/2	0.00	0.00	0.00	0.00	0.00	
3d ^{9 2} D	$3d_{-}^{3}3d_{+}^{6}$	(3/2,0)	3/2	537.21	538.04	538.59	535.6	538.05	

Table 3. Cont.

The uncertainties of NIST energy levels not based on observed wavelengths are estimated as being less than 5000 cm^{-1} , or 5.00 in our table. In order to better understand the importance of various effects in Table 4, we report the NIST energy levels that are based on observation and differences of various theories for only those levels where NIST values are accurate, although there may be an unknown shift.

Table 4. Difference from NIST energy levels derived from observation. Shown is the *LS* label, the *J* value, the present n = 5 result for VV correlation, and n = 6 result for all three types of correlation, the ASD value [5], the Quinet value [6], the Guo et al. RMBPT_g value [8], and the Safranova & Safronova RMBPT_s value [17]. All energy levels are reported in 1000 cm⁻¹.

Label	J	Presen $n = 5$	t Work $n = 6$	ASD	GRASP	RMBPT _g	RMBPT _s
W ⁵⁵	+ (K-lik	e)					
3d ² D	3/2	0.00	0.00	0.00	0.00	0.00	
$3d^2D$	5/2	1.25	0.32	626.49	2.49	-0.07	
W ⁵⁴⁻	+ (Ca-lil	ke)					
$3d^{2} {}^{3}F$	2	0.00	0.00	0.00	0.00	0.00	0.00
$3d^{2} {}^{3}F$	3	1.43	0.73	585.48	1.98	-0.32	2.63
3d ² ³ P	2	1.04	0.53	668.49	0.89	0.49	2.28
$3d^{2} {}^{3}P$	1	3.11	2.71	709.46+x	2.36	2.68	4.05
W ⁵³	+ (Sc-lik	ke)					
$3d^{3} {}^{4}F^{3}$	3/2	0.00	0.00	0.00	0.00	0.00	
$3d^{3} {}^{4}F^{3}$	5/2	1.64	0.96	530.03	1.83	-0.48	
$3d^{3} {}^{4}P^{3}$	3/2	1.43	0.87	580.86	0.96	0.0	
$3d^{3} {}^{4}P^{3}$	1/2	1.23	0.73	623.95	0.35	0.42	
$3d^{3} {}^{2}D^{1}$	5/2	0.38	0.15	812.22	-1.98	0.45	
$3d^{3} {}^{2}H^{3}$	11/2	1.13	0.21	1234.51+x	-1.69	0.45	
W ⁵²	+ (Ti-lik	xe)					
$3d^{4} {}^{3}P^{2}$	0	0.00	0.00	0.00	0.00	0.00	
$3d^{4} {}^{5}D^{4}$	1	1.76	1.12	517.63	1.63	-0.45	
$3d^{4} {}^{3}F^{2}$	3	-0.28	-0.53	665.5621+x	-3.04	-1.48	
$3d^{4} {}^{5}D^{4}$	2	2.87	1.71	1109.69	2.09	-0.33	
$3d^{4} \ ^{3}H^{4}$	4	1.73	0.68	1127.27+y	-0.03	-1.84	
$3d^{4} \ ^{3}H^{4}$	5	1.11	0.29	1173.35+y	-2.35	-22.25	
$3d^4 {}^3F^2$	4	0.29	-0.27	1403.95+x	-4.65	-1.16	
W ⁵¹	+ (V-lik	e)					
$3d^{5} {}^{4}P^{3}$	5/2	0.00	0.00	0.00	0.00	0.00	
$3d^{5} {}^{6}S^{5}$	5/2	1.92	0.88	471.63	2.53	-0.40	

Label	J	Presen $n = 5$	t Work $n = 6$	ASD	GRASP	RMBPT _g	RMBPT _s
$3d^{5} {}^{4}G^{5}$	7/2	1.27	0.45	566.25	0.05	-0.16	
$3d^{5} {}^{4}D^{5}$	3/2	1.28	0.39	580.89	1.09	0.45	
$3d^{5} {}^{2}F^{5}$	7/2	0.45	-0.10	688.18	-2.72	0.28	
$3d^{5} \ ^{4}G^{5}$	11/2	2.64	0.92	1103.43	0.43	-0.61	
W ⁵⁰	+ (Cr-lil	ke)					
$3d^{6} {}^{5}D^{4}$	4	0.00	0.00	0.00	0.00	0.00	
$3d^{6} {}^{3}D^{4}$	2	-0.36	-0.29	62.38	-0.22	0.82	
$3d^{6} {}^{5}D^{4}$	3	1.75	1.04	508.03	2.83	0.23	
$3d^{6} {}^{5}D^{4}$	4	1.41	0.74	519.78	1.78	0.05	
$3d^{6} {}^{3}G^{4}$	5	0.97	0.44	583.67	-0.53	-0.07	
$3d^{6} {}^{3}D^{4}$	3	1.15	0.56	650.91	0.31	1.09	
$3d^{6} {}^{3}P^{2}$	1	1.91	1.44	768.98+x	-0.32	2.60	
$3d^{6} {}^{3}D^{4}$	2	0.70	0.11	766.95	-0.65	1.26	
$3d^{6} {}^{1}G^{2}$	4	0.56	-0.04	761.21	-1.29	0.93	
$3d^{6} {}^{3}F^{2}$	3	0.35	-0.08	782.53	-2.47	1.27	
W ⁴⁹⁻	- (Mn-li	ke)					
$3d^{7} {}^{4}F^{3}$	9/2	0.00	0.00	0.00	0.00	0.00	
$3d^{7} {}^{2}D^{1}$	5/2	-0.20	-0.35	158.75	0.05	1.13	
$3d^{7} {}^{4}F^{3}$	7/2	1.68	0.78	529.66	3.56	0.58	
$3d^{7} {}^{4}F^{3}$	9/2	1.09	0.43	584.59	1.49	0.41	
$3d^{7} {}^{4}P^{3}$	5/2	3.05	2.30	628.02+x	3.12	2.61	
$3d^{7} {}^{4}P^{3}$	1/2	2.73	2.00	638.62+x	3.52	3.17	
$3d^{7} {}^{2}H^{3}$	11/2	0.54	0.12	650.70	-1.10	0.15	
$3d^{7} {}^{2}F^{3}$	7/2	0.72	0.21	705.92	-0.48	1.06	
W ⁴⁸	+ (Fe-lik	ke)					
3d ⁸ ³ F	4	0.00			0.00	0.00	0.00
3d ⁸ ³ F	3	1.47	0.58	526.65	3.45	0.52	
3d ^{8 3} P	2	2.74	1.97	603.12+x	3.42	2.43	
3d ^{8 3} P	1	2.73	2.05	644.76+x	2.06	2.62	
W ⁴⁷⁻	+ (Co-lil	ke)					
3d ⁹ ² D	5/2	0.00	0.00	0.00	0.00	0.00	
$3d^{9} {}^{2}D$	3/2	1.38	0.55	538.59	2.99	0.54	

Table 4. Cont.

Table 4 shows clearly that the uncertainties of the present n = 6 results are smaller by about a factor of a half when no shifts are indicated in the NIST value. For these levels, the n = 6 results statistically differ less than the Quinet values that are similar to the less accurate n = 5 values. The most accurate results for 3d and $3d^9$ are the RMCDHF_g results, although for $3d^9$, the n = 6 are almost of the same accuracy. RMBPT_g is the more accurate for $3d^2$, with n = 6 almost the same. For $3d^8$, the two lower levels, RMBPT_g is the more accurate, whereas n = 6 is the more accurate for the two upper levels. A similar pattern seems to hold for other spectra. An interesting case is $3d^7 \, ^4P \, J = 5/2$ and 1/2, where both levels have an unknown shift. An exact theoretical value and an exact NIST value (except for the shift) would have the same difference for the two levels. In the present case, the n = 6 differences are more similar than the RMCDHF_g differences. In fact, from this table, we can conclude that any NIST value for which the theoretical difference from NIST for both methods is more than 1.00

has a noticeable error. Thus, for example, the ${}^{3}P_{1}$ level of $3d^{8}$ with an energy level of 644.70 Kcm⁻¹ suggests that the NIST values is not accurate to two decimal places.

The errors in different theoretical results are shown in Figure 2. Note the similarity in accuracy of the present n = 6 results and values reported by Guo et al. [8].



Figure 2. Plot comparing the accuracy of different theoretical methods.

The accuracy of theoretical energy levels are best evaluated by comparing theoretical wavelengths with wavelengths of observed lines in the spectrum. In Table 5, all wavelengths for M1 transitions between the $3d^k$ levels for the present n = 5, 6 results are compared with experimental results and other theory, when available. This table clearly shows the improvement in accuracy of n = 6 calculations over n = 5, as well as the GRASP results reported by Quinet [6], and in many cases the very close agreement with Guo et al. [8]. Two exceptions are the $3d^7 \ ^2F^3$ (J = 9/2 to J = 7/2) transition, for which the observed wavelength is 14.166(3) nm, the present n = 6 is 14.170 nm, and the Guo et al. value is 14.187 nm. Similarly, the $3d^8 \ ^3F - 3d^8 \ ^1G$ (J = 4 to J = 4) transition has an observed wavelength of 15.511(3) nm, whereas the present value is 15.518 nm and the Guo et al. value is 15.463 nm.

Label a	nd J	Label a	and J	Present	Work	Expt	CRASP	RMRPT	RCI
for Lov	ver	for Up	pper	n = 5	n = 6	(Ref. [2])	GRASI	KWIDI Ig	KClg
W ⁵⁵⁺ (K-l	like)								
3 <i>d</i> ² <i>D</i>	3/2	3 <i>d</i> ² <i>D</i>	5/2	15.994	15.970	15.962(3)	16.008	15.960	16.035
W ⁵⁴⁺ (Ca	-like)								
$3d^{2} {}^{3}F$	2	$3d^{2} {}^{3}F$	3	17.122	17.101	17.080(3)	17.138	17.071	17.218
$3d^{2} {}^{3}F$	2	$3d^{2} {}^{3}P$	2	14.982	14.971	14.959(3)	14.980	14.970	14.924
$3d^{2} {}^{3}F$	2	$3d^{2} {}^{3}P$	1	14.157	14.149				
$3d^{2} {}^{3}F$	2	$3d^{2} {}^{3}P$	2	7.699	7.691				
$3d^{2} {}^{3}P$	0	$3d^{2} {}^{3}P$	1	19.233	19.211	19.177(3)	19.222	19.160	19.422
$3d^{2} {}^{3}F$	3	$3d^{2} {}^{3}P$	2	119.908	120.168				
$3d^{2} {}^{3}F$	3	$3d^{2} {}^{1}G$	4	89.580	89.805				
$3d^{2} {}^{3}F$	3	$3d^{2} {}^{3}F$	4	15.378	15.365				
$3d^{2} {}^{3}F$	3	$3d^{2} {}^{3}P$	2	13.989	13.977				
$3d^{2} {}^{3}P$	2	$3d^{2} {}^{3}P$	1	257.054	257.793				
$3d^{2} {}^{3}P$	2	$3d^{2} {}^{3}P$	2	15.836	15.817				
$3d^{2} {}^{3}P$	1	$3d^{2} {}^{3}P$	2	16.876	16.851				

Table 5. Wavelengths from theory for observed M1 transitions compared with observed wavelengths (in nm). Included are some long wavelengths for transitions between close-lying levels.

Label a	nd J	Label a	nd J	Presen	t Work	Expt	CD (CD		D.GT
for Lov	ver	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ^{2 3} P	1	3d ² ¹ S	0	12.728	12.707				
$3d^{2} {}^{1}G$	4	$3d^{2} {}^{3}F$	4	18.566	18.537				
W ⁵³⁺ (Sc-	like)								
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{4}F^{3}$	5/2	18.925	18.901	18.867(3)	18.933	18.850	19.120
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{4}P^{3}$	3/2	17.258	17.242	17.216(3)	17.243	17.216	17.315
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{4}P^{3}$	1/2	16.059	16.046	16.027(3)	16.035	16.038	16.038
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}D^{1}$	5/2	12.318	12.314	12.312(3)	12.282	12.319	12.225
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{4}P^{3}$	3/2	8.289	8.280				
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}P^{3}$	1/2	8.128	8.120				
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}D^{3}$	5/2	8.041	8.035				
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}F^{3}$	5/2	7.607	7.601				
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}D^{1}$	3/2	6.757	6.751				
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}P^{3}$	3/2	5.329	5.324				
$3d^{3} {}^{4}F^{3}$	3/2	$3d^{3} {}^{2}D^{1}$	5/2	5.107	5.102				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{4}P^{3}$	3/2	195.953	196.390				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}G^{3}$	7/2	121.923	122.264				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}D^{1}$	5/2	35.279	35.336				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{4}F^{3}$	7/2	16.697	16.680				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{4}P^{3}$	3/2	14.749	14.735				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}D^{3}$	5/2	13.981	13.975				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}F^{3}$	5/2	12.720	12.715				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}F^{3}$	7/2	12.654	12.651				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}D^{1}$	3/2	10.509	10.502				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}P^{3}$	3/2	7.418	7.412				
$3d^{3} {}^{4}F^{3}$	5/2	$3d^{3} {}^{2}D^{1}$	5/2	6.995	6.988				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{4}P^{3}$	1/2	230.965	231.304				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}D^{1}$	5/2	43.026	43.089				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{4}P^{3}$	3/2	15.949	15.930				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}P^{3}$	1/2	15.364	15.347				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}D^{3}$	5/2	15.055	15.046				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}F^{3}$	5/2	13.603	13.595				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}D^{1}$	3/2	11.105	11.095				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}P^{3}$	3/2	7.710	7.702				
$3d^{3} {}^{4}P^{3}$	3/2	$3d^{3} {}^{2}D^{1}$	5/2	7.254	7.246				
$3d^{3} {}^{2}H^{3}$	9/2	$3d^{3} {}^{2}G^{3}$	7/2	21322.871	18591.162				
$3d^{3} {}^{2}H^{3}$	9/2	$3d^{3} {}^{4}F^{3}$	7/2	19.329	19.295				
$3d^{3} {}^{2}H^{3}$	9/2	$3d^{3} {}^{4}F^{3}$	9/2	18.022	17.996				
$3d^{3}{}^{2}H^{3}$	9/2	$3d^{3} {}^{2}H^{3}$	11/2	15.812	15.798	15.785(3)	15.792	15.778	15.876
$3d^{3} {}^{2}H^{3}$	9/2	$3d^{3} {}^{2}F^{3}$	7/2	14.110	14.100				
$3d^{3}{}^{2}H^{3}$	9/2	$3d^{3} {}^{2}G^{3}$	9/2	8.673	8.661				
$3d^{3/2}G^{3}$	7/2	$3d^{3} {}^{2}D^{1}$	5/2	49.645	49.700				
$3d^{3/2}G^{3}$	7/2	$3d^{3} {}^{4}F^{3}$	7/2	19.346	19.315				
$3d^{3/2}G^{3}$	7/2	$3d^{3} {}^{4}F^{3}$	9/2	18.037	18.014				
$3d^{3/2}G^{3}$	7/2	$3d^{3} {}^{2}D^{3}$	5/2	15.791	15.779				
$3d^{3/2}G^{3}$	7/2	$3d^{3/2}F^{3}$	5/2	14.201	14.191				
$3d^{3} G^{3}$	7/2	$3d^{3} {}^{2}F^{3}$	7/2	14.119	14.110				
$3d^{3} + G^{3}$	7/2	$3d^{3} = 4G^{3}$	9/2	8.677	8.665				
$3d^3 \stackrel{2}{-} G^3$	7/2	$3d^{3} \stackrel{2}{=} D^{1}$	5/2	7.421	7.411				
3d° 4P°	1/2	3d ³ 4P ³	3/2	17.132	17.108				

Table 5. Cont.

Label a for Lo	nd J wer	Label a for Up	nd J per	Present $n = 5$	Work $n = 6$	Expt (Ref. [2])	GRASP	RMBPT _g	RCIg
2d3 4 p3	1/2	3d3 2p3	1/2	16 / 159	16 / 38				
$3d^3 4p^3$	1/2	$3d^{3} 2D^{1}$	3/2	11 665	11 654				
$3d^{3} 4p^{3}$	1/2	$3d^{3} 2p^{3}$	3/2	7 976	7 968				
$3d^{3} {}^{2}D^{1}$	5/2	$3d^{3} 4F^{3}$	7/2	31 700	31 592				
$3d^{3} 2D^{1}$	5/2	$3d^3 4p^3$	3/2	25 344	25 274				
$3d^{3} 2D^{1}$	5/2	$3d^{3} 2D^{3}$	5/2	23.157	23.274				
$3d^{3} 2D^{1}$	5/2	$3d^{3} 2E^{3}$	5/2	19 891	19 862				
$3d^{3} {}^{2}D^{1}$	5/2	$3d^{3} {}^{2}F^{3}$	7/2	19.730	19.705				
$3d^{3} 2D^{1}$	5/2	$3d^{3} {}^{2}D^{1}$	3/2	14 968	14 943				
$3d^{3} 2D^{1}$	5/2	$3d^{3} 2p^{3}$	3/2	9 393	9 379				
$3d^{3} 2D^{1}$	5/2	$3d^{3} 2D^{1}$	5/2	8 725	8 710				
$3d^{3} 4E^{3}$	7/2	$3d^3 4E^3$	9/2	266 613	267 118				
$3d^{3}4r^{3}$	7/2	3d ³ ² D ³	5/2	85 937	207. 11 0 86.197				
$3d^{3}4r^{3}$	7/2	$3d^{3} 2E^{3}$	5/2	53 397	53 / 92				
$3d^{3}4r^{3}$	7/2	$3d^{3} 2E^{3}$	7/2	52 253	52 370				
$3d^{3}4r^{3}$	7/2	$3d^{3} 2c^{3}$	9/2	15 733	15 717				
$3d^{3}4r^{3}$	7/2	$3d^{3} 2D^{1}$	5/2	12.038	12.026				
$3d^{3}4r^{3}$	9/2	3d ³ 2 H ³	$\frac{3}{2}$	12.050	12.020				
$3d^{3}4r^{3}$	9/2	$3d^{3} 2E^{3}$	$\frac{11}{2}$	6/ 991	65 122				
$3d^3 4 E^3$	9/2	$3d^{3} 2c^{3}$	9/2	16 719	16 608				
$3d^3 4 D^3$	3/2	$3^{3} 2^{3} 2^{3}$	9/2 1/2	10.719	10.090				
2 43 4 D3	3/2	2 d3 2 m3	1/2 5/2	410.403	419.220 271.110				
2 3 4 7	3/2	2432E3	5/2	200.399	02 751				
243403	2/2	$2432n^{1}$	3/2	92.443	92.731 26 EE0				
2 3 4 7	3/2	2 d3 2 D3	3/2	14 025	14 012				
243403	2/2	243201	5/2	14.923	14.912				
$2432 p^{3}$	3/2	$3u^3 - D^2$	3/2	13.305	13.291				
243203	1/2	24320^{-}	3/2	40.036	40.031				
2432113	1/2	$3u^{\circ} - P^{\circ}$	3/Z	10.477	10.402				
$3u^{\circ} = \Pi^{\circ}$	11/2 E/2	$3u^{\circ} - G^{\circ}$	9/2 E /2	19.211	19.173				
$2u^{3} - D^{2}$	5/2	$3u^{\circ} - F^{\circ}$	5/2	141.010	140.904				
$3a^{\circ} = D^{\circ}$	5/2	$3a^{\circ} - F^{\circ}$	2/2	133.312	133.450				
$3a^{\circ} = D^{\circ}$	5/2	$3a^{\circ} - D^{-}$	3/2	42.321	42.257				
$3a^{\circ} = D^{\circ}$	5/2	$3a^{\circ} - P^{\circ}$	3/2	15.804	12.07(
$3u^{2} - D^{2}$	5/2	$3u^{\circ} - D^{-}$	5/2	13.999	13.976				
$3a^{\circ} = F^{\circ}$	5/2	$3a^{\circ} - F^{\circ}$	2/2	2440.155	2497.085				
$3a^{\circ} = F^{\circ}$	5/2	$3a^{\circ} - D^{-}$	3/2	60.469	60.343				
$3u^{2} - F^{2}$	5/2	$3u^{2} - P^{2}$	5/2	17.798	17.769				
$3a^{\circ} = F^{\circ}$	5/2	$3a^{\circ} - D^{-}$	5/2	15.542	15.514				
$3a^{\circ} = F^{\circ}$	7/2	$3a^{\circ} - G^{\circ}$	9/2	22.510	22.456				
$3a^{\circ} = F^{\circ}$	2/2	$3a^{\circ} - D^{-}$	5/2	15.642	15.611				
$3a^{\circ} = D^{\circ}$	3/2	$3a^{\circ} - P^{\circ}$	3/2	25.222	25.185				
$3a^{2} D^{2}$	3/2	$3a^{\circ} - D^{1}$	5/2	20.919	20.883				
$3d^{5-2}P^{5-2}$	3/2	3d ⁵ ² D ¹	5/2	122.606	122.246				
$\frac{W^{32+}(1)}{24^{4} 3 R^{2}}$	·like)	0.14.5.54		10 205	10 2/1	10.010/2	10.050	10 000	10 (25
$3a^{+} SP^{-}$	0	$3a^{-5}D^{-1}$	1	19.385	19.361	19.319(3)	19.379	19.302	19.605
$3d^{\pm 5}P^{2}$	0	$3d^{+} {}^{3}D^{+}$	1	8.241	8.234				
$3d^{\pm 3}P^{2}$	0	$3d^{\pm 3}D^{\pm}$	1	5.660	5.654				
$3d^{\pm 5}P^{2}$	0	$3d^{-5}P^{2}$	1	5.041	5.037				
3d* ⁵ D*	1	3d4 ⁵ D4	2	81.888	82.053				

Table 5. Cont.

Label an	d J	Label an	d J	Present	Work	Expt	0.0.1.0.0	21/222	
for Low	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GRASP	RMBPTg	RCIg
3d ⁴ ⁵ D ⁴	1	$3d^{4} {}^{5}D^{4}$	0	17.065	17.045				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{5}D^{4}$	2	16.922	16.907	16.890(3)	16.903	16.894	16.958
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}D^{4}$	1	14.334	14.326				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}F^{4}$	2	13.479	13.475				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}F^{2}$	2	11.857	11.849				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4\ 1}D^2$	2	10.103	10.103				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}P^{4}$	0	8.950	8.947				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}D^{4}$	1	7.995	7.987				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}F^{4}$	2	7.545	7.539				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{1}S^{4}$	0	7.107	7.105				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}P^{2}$	1	6.812	6.808				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{1}D^{4}$	2	6.654	6.651				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{1}D^{2}$	2	5.142	5.137				
$3d^{4} {}^{5}D^{4}$	1	$3d^{4} {}^{3}P^{2}$	0	4.658	4.653				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	3	190.114	190.262				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}H^{4}$	4	19.520	19.491	19.445(3)	19.543	19.443	19.696
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{5}D^{4}$	3	18.912	18.886				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}H^{4}$	5	17.889	17.872	17.846(3)	17.855	17.831	18.065
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{4}$	3	15.977	15.965				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} \ {}^{3}G^{4}$	4	15.894	15.882				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	4	12.652	12.647				
$3d^{4} \ ^{3}H^{4}$	4	$3d^{4} {}^{5}D^{4}$	4	9.083	9.071				
$3d^{4} \ {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{4}$	3	8.993	8.981				
$3d^{4} \ {}^{3}H^{4}$	4	$3d^{4} \ {}^{3}G^{4}$	5	8.617	8.608				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} \ ^{3}D^{4}$	3	8.036	8.028				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	3	7.317	7.310				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{1}G^{2}$	4	7.290	7.283				
$3d^{4} \ {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	4	5.672	5.665				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{2}$	3	358.990	360.907				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{5}D^{4}$	2	21.329	21.295				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{5}D^{4}$	3	19.840	19.816				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}D^{4}$	1	17.375	17.356				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	3	16.635	16.624				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	2	16.135	16.123				
$3d^{4} {}^{5}D^{4}$	2	$3d^4 \ {}^3F^2$	2	13.864	13.849				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{1}D^{2}$	2	11.525	11.521				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	3	9.197	9.186				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}D^{4}$	1	8.860	8.848				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	2	8.311	8.302				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}D^{4}$	3	8.199	8.191				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{2}$	3	7.452	7.445				
$3d^{4} {}^{5}D^{4}$	2	$3d^4 \ ^3P^2$	1	7.430	7.424				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} D^{4}$	2	7.243	7.238				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4-1}D^2$	2	5.487	5.480				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{5}D^{4}$	2	22.677	22.630				
$3d^{4} {}^{5}F^{2}$	3	$3d^{4} {}^{3}H^{4}$	4	21.753	21.716				
$3d^{4} {}^{5}F^{2}$	3	$3d^{4} {}^{5}D^{4}$	3	21.001	20.968				
$3d^{\pm 3}F^{2}$	3	$3d^{\pm 3}F^{\pm}$	3	17.443	17.427				
$3d^{4} {}^{5}F^{2}$	3	$3d^{4} {}^{3}G^{4}$	4	17.344	17.329				
3d* 3F2	3	3d* 3F4	2	16.895	16.877				

Table 5. Cont.

Label and	11	Label an	d J	Present	Work	Expt	0.0.4.0.0		
for Lowe	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ⁴ ³ F ²	3	$3d^{4} {}^{3}F^{2}$	2	14.421	14.402				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}F^{2}$	4	13.554	13.548	13.543(3)	13.513	13.549	13.495
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}D^{2}$	2	11.907	11.901				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{5}D^{4}$	4	9.538	9.525				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}F^{4}$	3	9.439	9.426				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}F^{4}$	2	8.508	8.497				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}D^{4}$	3	8.390	8.381				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}F^{2}$	3	7.610	7.602				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}G^{2}$	4	7.581	7.573				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}D^{4}$	2	7.392	7.386				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}F^{2}$	4	5.847	5.839				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}D^{2}$	2	5.572	5.565				
$3d^{4} {}^{5}D^{4}$	0	$3d^{4} {}^{3}D^{4}$	1	89.555	89.798				
$3d^{4} {}^{5}D^{4}$	0	$3d^{4} {}^{3}D^{4}$	1	15.041	15.028				
$3d^{4} {}^{5}D^{4}$	0	$3d^{4} {}^{3}P^{2}$	1	11.338	11.334				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{5}D^{4}$	3	284.116	285.346				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}D^{4}$	1	93.723	93.840				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	3	75.583	75.791				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	2	66.257	66.382				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{2}$	2	39.611	39.610				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{1}D^{2}$	2	25.072	25.102				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	3	16.170	16.153				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}D^{4}$	1	15.154	15.138				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{4}$	2	13.617	13.605				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}D^{4}$	3	13.318	13.311				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}F^{2}$	3	11.453	11.448				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{3}P^{2}$	1	11.402	11.396				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{1}D^{4}$	2	10.967	10.964				
$3d^{4} {}^{5}D^{4}$	2	$3d^{4} {}^{1}D^{2}$	2	7.387	7.380				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{5}D^{4}$	3	606.876	608.761				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}H^{4}$	5	214.114	215.206				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{4}$	3	88.039	88.243				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}G^{4}$	4	85.561	85.781				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	4	35.956	36.020				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{5}D^{4}$	4	16.986	16.966				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{4}$	3	16.675	16.654				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}G^{4}$	5	15.427	15.416				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}D^{4}$	3	13.658	13.649				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	3	11.704	11.697				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{1}G^{2}$	4	11.635	11.628				
$3d^{4} {}^{3}H^{4}$	4	$3d^{4} {}^{3}F^{2}$	4	7.996	7.986				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}F^{4}$	3	102.978	103.203				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}G^{4}$	4	99.604	99.852				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}F^{4}$	2	86.407	86.507				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}F^{2}$	2	46.028	45.995				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}F^{2}$	4	38.221	38.285				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{1}D^{2}$	2	27.498	27.524				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{5}D^{4}$	4	17.475	17.453				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}F^{4}$	3	17.146	17.123				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{3}F^{4}$	2	14.303	14.287				

Table 5. Cont.

Label and	17	Label an	d <i>I</i>	Present	Work	Expt			
for Lowe	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d4 5D4	3	3,44 3,04	3	13 973	13 962				
$3d^{4} {}^{5} D^{4}$	3	$3d^{4} 3 E^{2}$	3	11 934	11 926				
$3d^{4} {}^{5}D^{4}$	3	$3d^{4} {}^{1}G^{2}$	4	11.204	11.920				
$3d^{4} {}^{5} D^{4}$	3	$3d^{4} {}^{1}D^{4}$	т 2	11.005	11.000				
$3d^{4} {}^{5} D^{4}$	3	$3d^{4} 3E^{2}$	4	8 102	8 092				
$3d^{4} {}^{5} D^{4}$	3	$3d^{4} D^{2}$	7 2	7 584	7 575				
3d ⁴ ³ H ⁴	5	$3d^{4} 1 l^{4}$	6	128 184	/30.120				
$3d^{4} {}^{3}H^{4}$	5	$3d^{4} {}^{3}C^{4}$	4	142 509	142 637				
$3d^{4} {}^{3} H^{4}$	5	$3d^{4} 3r^{2}$	т 4	43 213	43 261				
$3d^{4} {}^{3}H^{4}$	5	$3d^{4} {}^{5}D^{4}$	т 4	18 450	18 418				
$3d^{4} {}^{3}H^{4}$	5	$3d^{4} {}^{3}C^{4}$	5	16.625	16.605				
$3d^{4} {}^{3}H^{4}$	5	$3d^{4} {}^{3}H^{4}$	6	16.488	16.000				
$3d^{4} {}^{3}H^{4}$	5	$3d^{4} {}^{1}C^{2}$	4	12 304	12 292				
$3d^{4} {}^{3}H^{4}$	5	$3d^{4} 3E^{2}$	т 4	8 306	8 293				
$3d^{4} 1 I^{4}$	6	$3d^{4} {}^{3}C^{4}$	5	17 296	17 272				
$3d^{4}1t^{4}$	6	$3d^{4} \ ^{3} H^{4}$	6	17.290	17.272				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} 3F^{4}$	2	226.092	226 868				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} 3E^{2}$	2	68 606	68 5/1				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} {}^{1}D^{2}$	2	34 228	34 269				
$3d^{4} {}^{3} D^{4}$	1	$3d^{4} 3p^{4}$	0	23 832	23 832				
$3d^{4} {}^{3} D^{4}$	1	$3d^{4} {}^{3}D^{4}$	1	18 077	18 0/9				
$3d^{4} {}^{3}D^{4}$	1	3d4 3 F4	2	15 932	15.042				
$3d^{4} {}^{3} D^{4}$	1	3d4 1 54	0	14.097	1/ 09/				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} 3p^{2}$	1	12 981	12 972				
$3d^{4} {}^{3} D^{4}$	1	$3d4 \ 1D4$	2	12.001	12.772				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} 1D^{2}$	2	8 019	8 009				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} 3p^{2}$	0	6 900	6 892				
$3d^{4} {}^{3}E^{4}$	3	$3d^{4} {}^{3}C^{4}$	4	3040 724	3074 775				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} 3E^{4}$	2	536 990	534 715				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} 3E^{2}$	2	83 228	82 973				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} 3E^{2}$	4	60 779	60.864				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} D^{2}$	7 2	37 516	37 533				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{5}D^{4}$	4	21 047	21 005				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} 3E^{4}$	3	21.047	21.003				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} 3F^{4}$	2	16 610	16 582				
$3d^{4} {}^{3}E^{4}$	3	$3d^{4} {}^{3}D^{4}$	2	16.010	16.147				
$3d^{4} {}^{3}E^{4}$	3	$3d^{4} 3E^{2}$	3	13 498	13 485				
$3d^{4} {}^{3}E^{4}$	3	$3d^{4} {}^{1}C^{2}$	4	13.407	13 393				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{1}D^{4}$	2	12 829	12 819				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{3}F^{2}$	4	8 794	8 780				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{1}D^{2}$	2	8 187	8 176				
$3d^{4} {}^{3}G^{4}$	4	$3d^{4} {}^{3}F^{2}$	4	62 019	62 093				
$3d^{4} {}^{3}G^{4}$	1 1	$3d^{4} {}^{5}D^{4}$	4	21 194	21 149				
$3d^{4} {}^{3}G^{4}$	1 1	$3d^{4} {}^{3}F^{4}$	3	20.711	21.147				
$3d^{4} {}^{3}G^{4}$	1 1	$3d^{4} {}^{3}C^{4}$	5	18 820	18 793				
$3d^{4} {}^{3}G^{4}$	4	$3d^{4} {}^{3}D^{4}$	3	16 253	16 232				
$3d^{4} {}^{3}G^{4}$	4	$3d^{4} {}^{3}F^{2}$	3	13.559	13.544				
$3d^{4} {}^{3}G^{4}$	4	$3d^{4} {}^{1}G^{2}$	4	13 466	13 452				
$3d^{4} {}^{3}G^{4}$	4	$3d^{4} {}^{3}F^{2}$	4	8.820	8.805				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{3}F^{2}$	2	98,494	98.213				

Table 5. Cont.

Label and	17	Label an	d I	Present	Work	Expt			
for Lowe	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d4 3F4	2	3d ⁴ ¹ D ²	2	40 334	40 367				
3d4 3 F4	2	3d4 3 E4	2	21 391	21 348				
$3d^{4} 3F^{4}$	2	$3d^{4} {}^{3}D^{4}$	1	19 648	19 609				
$3d^{4} 3F^{4}$	2	$3d^{4} {}^{3}E^{4}$	2	17.010	17 113				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} \ {}^{3}D^{4}$	2	16 668	16 649				
$3d^{4} 3F^{4}$	2	$3d^{4} {}^{3}E^{2}$	3	13.846	13 834				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} 3p^{2}$	1	13.040	13 759				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{1}D^{4}$	2	13.143	13 133				
$3d^{4} 3F^{4}$	2	$3d^{4} {}^{1}D^{2}$	2	8 314	8 302				
$3d^{4} {}^{3}F^{2}$	2	$3d^{4} {}^{1}D^{2}$	2	68 306	68 536				
$3d^{4} 3F^{2}$	2	$3d^{4} {}^{3}E^{4}$	2	27 325	27 278				
$3d^{4} 3E^{2}$	2	$3d^{4} {}^{3}D^{4}$	1	24 544	24 501				
$3d^{4} 3F^{2}$	2	$3d^{4} {}^{3}E^{4}$	2	20.751	24.001				
$3d^{4} 3F^{2}$	2	$3d^{4} {}^{3}D^{4}$	2	20.751	20.724				
$3d^{4} 3F^{2}$	2	$3d^{4} {}^{3}E^{2}$	3	16 111	16 102				
$3d^{4} 3F^{2}$	2	$3d^{4} 3p^{2}$	1	16.011	16,000				
$3d^{4} 3E^{2}$	2	$3d^{4} D^{4}$	2	15 166	15 161				
$3d^{4} 3E^{2}$	2	$3d^{4} D^{2}$	2	9.081	9.069				
$3d^{4} 3E^{2}$	4	$3d^{4} 5D^{4}$	4	32 196	32 074				
$3d^{4} 3E^{2}$	+ 1	$3d^{4} 3t^{4}$	- 4	31.096	30.977				
$3d^{4} 3E^{2}$	+ 1	$3d^{4} \ ^{3}C^{4}$	5	27 020	26.950				
$3443E^2$	+ 1	3d4 3D4	3	27.020	20.950				
$3443E^2$	+ 1	$3d4 3 E^2$	3	17 352	17 323				
$3443E^2$	+ 1	$3d4 \ 1C^2$	4	17.332	17.525				
$3443E^2$	+ 1	$3d4 3 E^2$	4	10 282	10.260				
$3d4 \ 1 D^2$	+ 2	3d4 3E4	- 4	10.202	10.200				
$3d^{4} 1D^{2}$	2	3d4 3D4	1	38 310	40.01Z				
$3d^{4} 1D^{2}$	2	3d4 3E4	1	29.806	20 706				
$3d^{4} 1D^{2}$	2	3d4 3D4	2	29.800	29.700				
$3d^{4} D^{2}$	2	3d4 3E2	3	20.407	20.007				
$3d^{4} D^{2}$	2	$3d^{4} 3p^{2}$	1	21.005	21.040				
$3d^{4} D^{2}$	2	$3d^{4} 1 D^{4}$	1	10.912	20.075				
$3d^{4} D^{2}$	2	$3d^{4} D^{2}$	2	19.495	19.407				
$3d^{4} 3d^{4}$	0	$3d^{4} {}^{3}D^{4}$	2 1	74 865	74 385				
$3d^{4} 3p^{4}$	0	$3d^{4} 3p^{2}$	1	74.000 28 511	74.000 28.466				
$3d^{4} 5D^{4}$	4	$3d^{4} 3E^{4}$	3	910.088	905 530				
$3d^{4} 5D^{4}$	т 1	$3d^{4} {}^{3}C^{4}$	5	168.067	168 682				
$3d^{4} 5D^{4}$	т 1	$3d^{4} {}^{3}D^{4}$	3	69 712	69.810				
$3d^{4} {}^{5}D^{4}$	т 4	$3d^{4} {}^{3}E^{2}$	3	37.636	37.665				
$3d^{4} {}^{5}D^{4}$	т 4	$3d^{4} {}^{1}C^{2}$	4	36 935	36 959				
$3d^{4} {}^{5}D^{4}$	т 4	$3d^{4} {}^{3}E^{2}$	4	15 106	15.086				
$3d^{4} 3E^{4}$	т 3	$3d^{4} 3E^{4}$	- - 2	86 253	86 253				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{3}D^{4}$	∠ ג	75 495	75 642				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{3}F^{2}$	3	39 260	39 300				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{1}C^{2}$	4	38 498	38 532				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{1}D^{4}$	- 2	34 085	34 130				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{3}F^{2}$	4	15 361	15 342				
$3d^{4} {}^{3}F^{4}$	3	$3d^{4} {}^{1}D^{2}$	2	13 600	13 586				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} {}^{3}F^{4}$	2	134 268	134 420				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} {}^{1}S^{4}$	0	64.031	64.317				

Table 5. Cont.

Label a	nd J	Label aı	nd I	Present	Work	Expt			
for Lov	ver	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ⁴ ³ D ⁴	1	3d ⁴ ³ p ²	- 1	46 049	46 113				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} {}^{1}D^{4}$	2	39.694	39.769				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} {}^{1}D^{2}$	2	14 413	14.399				
$3d^{4} {}^{3}D^{4}$	1	$3d^{4} {}^{3} P^{2}$	0	11 160	11 149				
$3d^{4} {}^{3}G^{4}$	5	$3d^{4} {}^{3}H^{4}$	6	1997 212	2027 160				
$3d^{4} {}^{3}G^{4}$	5	$3d^{4} {}^{1}G^{2}$	4	47.338	47.329				
$3d^{4} {}^{3}G^{4}$	5	$3d^{4} {}^{3}F^{2}$	4	16.598	16.568				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{3}D^{4}$	3	605.307	614.828				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{3}F^{2}$	3	72.059	72.193				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{3}P^{2}$	1	70.085	70.193				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{1}D^{4}$	2	56.355	56.479				
$3d^{4} {}^{3}F^{4}$	2	$3d^{4} {}^{1}D^{2}$	2	16.146	16.126				
$3d^{4} {}^{3}D^{4}$	3	$3d^{4} {}^{3}F^{2}$	3	81.796	81.797				
$3d^{4} {}^{3}D^{4}$	3	$3d^{4} {}^{1}G^{2}$	4	78.556	78.539				
$3d^{4} {}^{3}D^{4}$	3	$3d^{4} {}^{1}D^{4}$	2	62.140	62.192				
$3d^{4} {}^{3}D^{4}$	3	$3d^{4} {}^{3}F^{2}$	4	19.285	19.245				
$3d^{4} {}^{3}D^{4}$	3	$3d^{4} {}^{1}D^{2}$	2	16.589	16.561				
$3d^{4} {}^{1}S^{4}$	0	$3d^{4} {}^{3}P^{2}$	1	163.968	162.926				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}G^{2}$	4	1982.892	1971.659				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}D^{4}$	2	258.586	259.474				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{3}F^{2}$	4	25.235	25.166				
$3d^{4} {}^{3}F^{2}$	3	$3d^{4} {}^{1}D^{2}$	2	20.809	20.765				
$3d^{4} {}^{3}P^{2}$	1	$3d^{4} {}^{1}D^{4}$	2	287.662	289.068				
$3d^{4} {}^{3}P^{2}$	1	$3d^{4} {}^{1}D^{2}$	2	20.980	20.936				
$3d^{4} {}^{3}P^{2}$	1	$3d^{4} {}^{3}P^{2}$	0	14.730	14.704				
$3d^{4} {}^{1}G^{2}$	4	$3d^{4} {}^{3}F^{2}$	4	25.560	25.491				
$3d^{4} \ ^{1}D^{4}$	2	$3d^{4} {}^{1}D^{2}$	2	22.630	22.571				
W ⁵¹⁺ (V-1	ike)								
		0 15 6 65	E /0	01 000	01.040	01.000(0)	21.015	01 105	01.400
$3d^{5} + P^{5}$	5/2	$3d^{5} + 5^{5}$	5/2	21.290	21.243	21.203(3)	21.317	21.185	21.492
$3a^{\circ} P^{\circ}$	5/2	$3a^{\circ} + G^{\circ}$	7/2	17.700	17.674	17.660(3)	17.660	17.655	17.826
$3a^{5} + P^{5}$	5/2	$3a^{5} + D^{5}$	3/2	17.253	17.227	17.215(3)	17.247	17.228	17.249
$3a^{\circ} P^{\circ}$	5/2	$3a^{\circ} D^{\circ}$	5/2	15.368	15.350	14 501(0)	14 475	14 525	14 510
$3a^{\circ} P^{\circ}$	5/2	$3a^{\circ} = F^{\circ}$	2/2	14.541	14.529	14.531(3)	14.475	14.537	14.513
$3u^{\circ} P^{\circ}$	5/2	30° - D- 245 6 c5	5/2	12.136	0.729				
$3u^{\circ} P^{\circ}$	5/2	30° °5°	5/2	9.747	9.728				
$3u^{\circ} P^{\circ}$	5/2	$3u^{\circ} D^{\circ}$	2/2	9.117	9.102				
2 45 4 p3	5/2	30° 1 P° 245 2 E5	5/2	0.000 0.511	8.571				
$3u^{\circ} P^{\circ}$	5/2	$3u^{\circ} = F^{\circ}$	5/2	8.511	8.499				
$3u^{2} - P^{2}$	5/2	$3u^{2} - G^{2}$	7/2 E /2	8.078 7.071	8.068 7.050				
$3u^{2} - P^{2}$	5/2	$3u^{-}F^{-}$	3/2	7.971	7.939				
$2454 P^{3}$	5/2	$3u^{2} = D^{2}$	3/2	7.940	7.931				
$5u^{-1}P^{-2}$ 2,45 4 p3	5/2	5u ² = G ² 2 d5 2 n3	2/2	7.040 6.645	7.030				
$2454n^{3}$	5/2	$5u^2 = P^2$ $2 J_2 = 2 J_2$	5/2	0.040	0.039				
2454n3	5/2	2 d5 4 n3	5/2	0.32Z	0.010				
2454n3	5/2	2454r3	5/2	0.021 E 760	0.010 E 750				
зи Р 2,454 пЗ	5/2	3d5 4D5	2/2	5.700	5.758				
$3u^{54}D^{3}$	5/2	3d5 2m3	5/2	5.004	5.074				
<i>Jn 1</i>				J. + 4 +	0.410				

Table 5. Cont.

Label a	nd J	Label a	nd I	Present	Work	Expt			
for Lo	wer	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
$3d^{5} 4 P^{3}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	4.847	4.841				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^{5} {}^{2}D^{1}$	5/2	4.233	4.225				
3d ⁵ 6S ⁵	5/2	$3d^{5} {}^{4}G^{5}$	7/2	104.969	105.214				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{4}D^{5}$	3/2	90.995	91,119				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{4}D^{5}$	5/2	55.250	55.341				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}F^{5}$	7/2	45.868	45.971				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	28.226	28.233				
3d ^{5 6} S ⁵	5/2	$3d^{5} {}^{6}S^{5}$	5/2	17.977	17.946				
3d ^{5 6} S ⁵	5/2	$3d^{5} {}^{4}D^{5}$	7/2	15.946	15.927				
3d ^{5 6} S ⁵	5/2	$3d^{5} {}^{4}P^{3}$	3/2	14.388	14.367				
3d ^{5 6} S ⁵	5/2	$3d^{5} {}^{2}F^{5}$	5/2	14.181	14.167				
3d ^{5 6} S ⁵	5/2	$3d^{5} {}^{2}G^{5}$	7/2	13.018	13.009				
3d ^{5 6} S ⁵	5/2	$3d^{5} {}^{4}F^{3}$	5/2	12.741	12.727				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}D^{5}$	3/2	12.662	12.655				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}G^{3}$	7/2	11.932	11.921				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}P^{3}$	3/2	9.660	9.657				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}D^{1}$	5/2	9.403	9.399				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{4}P^{3}$	5/2	8.395	8.381				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{4}F^{3}$	7/2	7.912	7.900				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{4}D^{5}$	3/2	7.755	7.743				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}D^{3}$	5/2	7.277	7.269				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}G^{3}$	7/2	7.133	7.124				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	6.276	6.269				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} {}^{2}D^{1}$	5/2	5.283	5.274				
$3d^{5} \ ^{4}G^{5}$	7/2	$3d^{5} {}^{2}G^{5}$	9/2	178.750	179.156				
$3d^{5} \ ^{4}G^{5}$	7/2	$3d^5 \ ^4D^5$	5/2	116.648	116.752				
$3d^{5} \ ^{4}G^{5}$	7/2	$3d^{5} {}^{2}F^{5}$	7/2	81.465	81.645				
$3d^{5} \ ^{4}G^{5}$	7/2	$3d^{5} {}^{6}S^{5}$	5/2	21.692	21.637				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{4}D^{5}$	7/2	18.802	18.768				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} \ ^{4}G^{5}$	9/2	18.116	18.086				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{2}F^{5}$	5/2	16.396	16.372				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{2}H^{3}$	9/2	15.329	15.304				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{2}G^{5}$	7/2	14.861	14.845				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{4}F^{3}$	5/2	14.501	14.479				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{2}G^{3}$	7/2	13.462	13.444				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{2}G^{3}$	9/2	12.275	12.264				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	10.329	10.321				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{4}P^{3}$	5/2	9.125	9.106				
$3d^{5} {}^{4}G^{5}$	7/2	$3d^{5} {}^{4}F^{3}$	7/2	8.557	8.541				
$3d^{5} {}^{4}G^{5}$	7/2	3d ^{5 2} G ⁵	9/2	8.057	8.044				
$3d^5 {}^4G^5$	7/2	$3d^{5} {}^{2}D^{3}$	5/2	7.820	7.808				
$3d^5 {}^4G^5$	7/2	$3d^{5} {}^{2}G^{3}$	7/2	7.653	7.642				
$3d^5 \ {}^4G^5$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	5.563	5.553				
$3d^{5}{}^{2}H^{3}$	11/2	$3d^{5} {}^{2}G^{5}$	9/2	222.726	223.030				
$3d^{5}{}^{2}H^{3}$	11/2	$3d^{5} {}^{4}G^{5}$	11/2	19.056	19.021	18.996(3)	19.064	19.002	19.185
$3d^{5}{}^{2}H^{3}$	11/2	$3d^5 {}^4G^5$	9/2	18.486	18.453				
$3d^{5}{}^{2}H^{3}$	11/2	$3d^{5/2}I^{5}$	13/2	17.664	17.637				
$3d^{5/2}H^{3}$	11/2	$3d^{5/2}H^{3}$	9/2	15.593	15.566				
$3d^{5}{}^{2}H^{3}$	11/2	$3d^{5} {}^{2}G^{3}$	9/2	12.443	12.432				
3d ^{5 2} H ³	11/2	3d ^{5 2} H ³	11/2	8.544	8.528				

Table 5. Cont.

Label a	nd J	Label a	nd J	Present	Work	Expt	0.0.4.0.0		
for Lo	wer	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
$3d^{5} {}^{2}H^{3}$	11/2	$3d^{5} {}^{2}G^{5}$	9/2	8.129	8.116				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}D^{5}$	5/2	140.653	140.944				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}P^{3}$	1/2	100.009	100.120				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{2}D^{1}$	3/2	40.920	40.907				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{6}S^{5}$	5/2	22.403	22.348				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}D^{5}$	1/2	17.360	17.334				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}P^{3}$	3/2	17.091	17.056				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{2}F^{5}$	5/2	16.799	16.775				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}F^{3}$	5/2	14.815	14.794				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{2}D^{5}$	3/2	14.708	14.696				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}P^{3}$	1/2	13.725	13.709				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{2}P^{3}$	3/2	10.807	10.802				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	10.487	10.480				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{4}P^{3}$	5/2	9.248	9.230				
$3d^5 \ ^4D^5$	3/2	$3d^5 \ ^4D^5$	3/2	8.477	8.462				
$3d^{5} {}^{4}D^{5}$	3/2	$3d^{5} {}^{2}D^{3}$	5/2	7.910	7.899				
$3d^5 \ ^4D^5$	3/2	$3d^{5} {}^{2}P^{3}$	1/2	7.384	7.375				
$3d^5 \ ^4D^5$	3/2	$3d^{5} {}^{2}D^{1}$	3/2	6.741	6.733				
$3d^5 \ ^4D^5$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	5.609	5.598				
3d ^{5 2} G ⁵	9/2	$3d^{5} {}^{2}F^{5}$	7/2	149.683	150.005				
3d ^{5 2} G ⁵	9/2	$3d^5 \ ^4D^5$	7/2	21.012	20.964				
3d ^{5 2} G ⁵	9/2	$3d^5 \ ^4G^5$	11/2	20.839	20.795				
3d ^{5 2} G ⁵	9/2	$3d^5 \ ^4G^5$	9/2	20.159	20.117				
3d ^{5 2} G ⁵	9/2	3d ^{5 2} H ³	9/2	16.767	16.734				
3d ^{5 2} G ⁵	9/2	3d ⁵ ² G ⁵	7/2	16.209	16.186				
3d ^{5 2} G ⁵	9/2	$3d^{5} {}^{2}G^{3}$	7/2	14.558	14.535				
$3d^{5} {}^{2}G^{5}$	9/2	$3d^{5} {}^{2}G^{3}$	9/2	13.180	13.165				
$3d^{5} {}^{2}G^{5}$	9/2	$3d^5 \ {}^4F^3$	7/2	8.987	8.969				
$3d^{5} {}^{2}G^{5}$	9/2	$3d^{5} {}^{2}H^{3}$	11/2	8.885	8.867				
$3d^{5} {}^{2}G^{5}$	9/2	$3d^{5} {}^{2}G^{5}$	9/2	8.437	8.422				
$3d^{5} {}^{2}G^{5}$	9/2	$3d^{5} {}^{2}G^{3}$	7/2	7.995	7.982				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} {}^{2}F^{5}$	7/2	270.094	271.516				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5/2}D^{1}$	3/2	57.709	57.636				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} {}^{6}S^{5}$	5/2	26.647	26.559				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} {}^{4}D^{5}$	7/2	22.415	22.363				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} {}^{4}P^{3}$	3/2	19.454	19.404				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} {}^{2}F^{5}$	5/2	19.077	19.042				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} = G^{5}$	7/2	17.031	17.007				
$3d^{5} {}^{4}D^{5}$	5/2	$3d^{5} = F^{3}$	5/2	16.560	16.529				
$3d^{5} = 4D^{5}$	5/2	$3d^{5} {}^{2}D^{5}$	3/2	16.426	16.407				
$3d^{5} = 4D^{5}$	5/2	$3d^{5/2}G^{5}$	7/2	15.218	15.194				
$3d^{5} + D^{5}$	5/2	$3d^{5} = 2P^{5}$	3/2	11.706	11.699				
$3d^{3} + D^{3}$	5/2	$3d^{5} + D^{1}$	5/2	11.332	11.322				
$3d^{5} + D^{5}$	5/2	$3d^{5} + P^{5}$	5/2	9.899	9.876				
$3d^{5} + D^{5}$	5/2	$3d^{5} + F^{5}$	7/2	9.234	9.215				
$3d^{5} = D^{5}$	5/2	$3d^{5} = D^{5}$	3/2	9.021	9.002				
$3d^{3} = D^{3}$	5/2	$3d^{3} + D^{3}$	5/2	8.381	8.368				
$3a^{5} = D^{5}$	5/2	$3a^{5} - G^{5}$	7/2	8.190	8.177				
$3d^{5} + D^{5}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	7.080	7.070				
$3a^{3} * D^{3}$	5/2	$3a^{3} 2D^{1}$	5/2	5.842	5.830				

Table 5. Cont.

Label a	nd J	Label a	nd J	Present	Work	Expt	00400		D .07
for Lov	ver	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPTg	RCIg
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}D^{1}$	3/2	69.257	69.169				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{4}D^{5}$	1/2	21.006	20.963				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{4}P^{3}$	3/2	20.613	20.559				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}D^{5}$	3/2	17.245	17.225				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{4}P^{3}$	1/2	15.909	15.884				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}P^{3}$	3/2	12.116	12.109				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{4}D^{5}$	3/2	9.262	9.243				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}P^{3}$	1/2	7.973	7.962				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}D^{1}$	3/2	7.228	7.218				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{6}S^{5}$	5/2	29.564	29.438				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{4}D^{5}$	7/2	24.443	24.370				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{4}G^{5}$	9/2	23.296	23.233				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}F^{5}$	5/2	20.527	20.478				
$3d^{5} {}^{2}F^{5}$	7/2	3d ^{5 2} H ³	9/2	18.882	18.835				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}G^{5}$	7/2	18.177	18.143				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{4}F^{3}$	5/2	17.641	17.600				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}G^{3}$	7/2	16.127	16.094				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}G^{3}$	9/2	14.452	14.432				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	11.828	11.814				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{4}P^{3}$	5/2	10.275	10.249				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{4}F^{3}$	7/2	9.561	9.539				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}G^{5}$	9/2	8.941	8.923				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}D^{3}$	5/2	8.650	8.634				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}G^{3}$	7/2	8.446	8.431				
$3d^{5} {}^{2}F^{5}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	5.971	5.958				
$3d^{5} {}^{2}D^{1}$	3/2	3d ^{5 6} S ⁵	5/2	49.507	49.256				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^5 \ ^4D^5$	1/2	30.151	30.080				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^5 {}^4P^3$	3/2	29.348	29.253				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5} {}^{2}F^{5}$	5/2	28.498	28.437				
$3d^{5/2}D^{1}$	3/2	$3d^{5} {}^{4}F^{3}$	5/2	23.224	23.175				
$3d^{5/2}D^{1}$	3/2	$3d^{5} {}^{2}D^{5}$	3/2	22.962	22.936				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5} {}^{4}P^{3}$	1/2	20.653	20.619				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5} {}^{2}P^{3}$	3/2	14.685	14.678				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	14.101	14.089				
$3d^{5-2}D^{1}$	3/2	$3d^{5} = P^{5}$	5/2	11.948	11.919				
$3d^{5-2}D^{1}$	3/2	$3d^{5} = D^{5}$	3/2	10.692	10.668				
$3d^{5} = D^{1}$	3/2	$3d^{5} + D^{5}$	5/2	9.806	9.789				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5} = P^{5}$	1/2	9.010	8.997				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5-2}D^{1}$	3/2	8.071	8.059				
$3d^{5} = D^{1}$	3/2	$3d^{5} = D^{1}$	5/2	6.500	6.486				
$3d^{5} {}^{6}S^{5}$	5/2	$3d^{5} = D^{5}$	7/2	141.121	141.559				
$3d^{5} \circ S^{5}$	5/2	$3d^{5} + P^{5}$	3/2	72.074	72.035				
$3d^{5} \circ S^{5}$	5/2	$3d^{5} + F^{5}$	5/2	67.156	67.278				
$3a^{5}$ $^{6}S^{5}$	5/2	$3a^{5} + G^{5}$	7/2	47.192	47.288				
$3a^{5}$ $^{6}S^{5}$	5/2	$3a^{5} = F^{5}$	5/2	43.743	43.766				
$3a^{5}$ $^{6}S^{5}$	5/2	$3a^{5} + D^{5}$	3/2	42.824	42.924				
30 050	5/2	$3a^{5} - G^{5}$	7/2	35.481	35.505				
3a° ° 5° 245.665	5/2 E/2	$3a^{5} - P^{5}$	3/2	20.879	20.910				
3a° °5° 245.665	5/2	$3a^{\circ} - D^{\circ}$	5/2	19.717	19.734				
3u~ °S°	3/2	50° 1P°	5/2	15./49	15.723				

Table 5. Cont.

Label a	nd I	Label a	nd I	Present	Work	Expt			
for Lo	wer	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
2.45.6.65	E /2	2.45.4 53	7/2	14 120	1/111				
30° ° 5° 245 6 65	5/2	$3u^{\circ} + F^{\circ}$	2/2	14.130	14.111				
2456c5	5/2	2 d5 2 D3	5/2	12.038	10.010				
3u ² 3 ² 2 45 6 c5	5/2	$2452C^{3}$	7/2	12.227	12.217				
30° ° 5° 245 665	5/2	$3u^{\circ} - G^{\circ}$	2/2	0.642	11.815				
3u ² 5 ² 2 45 6 c5	5/2	24520^{1}	5/2	9.043	9.030				
2 d ⁵ 4 D ⁵	5/2	$2454C^{5}$	5/Z	7.402 406 E49	7.470				
2 d ⁵ 4 D ⁵	7/2	$3u^{2}$ G^{2}	9/Z 5/2	490.340	497.001				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - F^{\circ}$	5/2	128.131	128.214				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - H^{\circ}$	9/2	82.993	82.924 71.000				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - G^{\circ}$	7/2 E/2	70.903	/1.009				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - F^{\circ}$	5/2	63.393	63.333				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - G^{\circ}$	0/2	47.397	47.392				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - G^{\circ}$	9/2 E/2	35.359	33.390				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - D^{-}$	5/2	22.919	22.931				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - P^{\circ}$	5/2	17.728	17.000				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - F^{\circ}$	0/2	15.703	13.674				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - G^{\circ}$	9/2 E/2	12.097	14.078				
$3u^{\circ} - D^{\circ}$	7/2	$3u^{\circ} - D^{\circ}$	5/2	13.387	13.371				
$3a^{\circ} D^{\circ}$	7/2	$3a^{\circ} - G^{\circ}$	7/2	12.906	12.891				
$3a^{\circ} D^{\circ}$	11/2	$3a^{\circ} - D^{\circ}$	5/2	7.901	/.886				
$3a^{\circ} + G^{\circ}$	11/2	$3a^{\circ}$ $^{\circ}$ G°	9/2	617.468	617.572				
$3a^{\circ} + G^{\circ}$	11/2	$3a^{\circ} - 1^{\circ}$	13/2	241.792	242.297				
$3a^{\circ} + G^{\circ}$	11/2	$3a^{\circ} - H^{\circ}$	9/2	85.801	85.691				
$3u^{\circ} + G^{\circ}$	11/2	$3a^{\circ} - G^{\circ}$	9/2	33.839 15.499	33.883 15.460				
$3u^{\circ} + G^{\circ}$	11/2	$3u^{\circ} - H^{\circ}$	0/2	13.488	13.460				
$3u^{\circ} + G^{\circ}$	0/2	$3a^{\circ} - G^{\circ}$	9/2	14.176	14.155				
$3u^{\circ} + G^{\circ}$	9/2	$3u^{\circ} - H^{\circ}$	9/2	99.648	99.490				
$3u^{\circ} + G^{\circ}$	9/2	$3a^{\circ} - G^{\circ}$	7/2	82.713 52.200	02.022 50.079				
$3u^{\circ} - G^{\circ}$	9/2	$3u^{\circ} - G^{\circ}$	0/2	32.399	32.370 28.000				
$3u^{\circ} - G^{\circ}$	9/2	$3u^{\circ} - G^{\circ}$	9/2	36.069	30.090				
$3u^{\circ} - G^{\circ}$	9/2	30° - F° 245 2113	11/2	16.215	10.103				
$3u^{\circ} - G^{\circ}$	9/2	$3u^{\circ} - H^{\circ}$	0/2	13.887	13.837				
$3u^{\circ} - G^{\circ}$	9/2	$3u^{\circ} - G^{\circ}$	9/2	14.509	14.48/				
30° G° 245 215	9/2	$3u^{\circ} - G^{\circ}$	11/2	13.250	15.255 16 E12				
$3u^{\circ} - 1^{\circ}$ $2u^{5} 4 D^{5}$	13/2	зи° - н° 2 45 4 р3	2/2	10.548	10.515				
$3u^{\circ} - D^{\circ}$ $2u^{5} 4 D^{5}$	1/2	$3u^{\circ} - P^{\circ}$	3/2	06 207	1064.996				
2 d ⁵ 4 D ⁵	1/2	$2 45 4 \mu^3$	3/2	90.307 65 560	90.303 65 562				
2 d ⁵ 4 D ⁵	1/2	$2452n^3$	1/2	03.300	00.002				
2 d ⁵ 4 D ⁵	1/2	2 d5 4 D5	3/2	26.630	20.000				
2 d ⁵ 4 D ⁵	1/2	$2 45 2 m^{3}$	3/2	10.300	10.002				
2 d ⁵ 4 D ⁵	1/2	245201	1/2	12.049	12.007				
2454 m^3	1/2	2452r5	5/2	11.021	1019 757				
345 4 D3	3/2	3d5 4r3	5/2	704.17/ 111 201	1010./3/				
345 4 D3	3/2	3d5 2m5	3/2	111.204	111.020				
345 4 D3	3/2	3d5 4 D3	5/Z	40 704	60.062				
345 4 D3	3/2	зи Р 2,45 2 рЗ	1/Z	09.704 20.202	20 161				
345 4 D3	3/2	3d5 2n1	5/2	27.373 27 1.11	27.401 27.100				
зи г 3,454 D3	3/2	3d5 4 D3	5/2	27.141	27.100				
$3d^{5} 4p^{3}$	3/2	$3d^{5} {}^{4}D^{5}$	3/2	16 820	16 793				

Table 5. Cont.

Label a	nd I	Label a	nd I	Present	Work	Expt			
for Lov	ver	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
2 d5 4 D3	3/7	3d5 2D3	5/2	14 726	14 712				
$3d^5 4 p^3$	3/2	3d5 2 p3	1/2	14.720	14.712				
$3d^{5} 4p^{3}$	3/2	$3d^{5} 2D^{1}$	$\frac{1}{2}$	11 132	12.774				
$3d^5 4 p^3$	3/2	$3d^{5} 2D^{1}$	5/2	8 3/0	8 33/				
$3d^{5}2t^{5}$	5/2	$3d^{5} 2c^{5}$	7/2	158 747	150 155				
$3d^{5} 2E^{5}$	5/2	$3d^5 4 E^3$	5/2	125 471	125 234				
$3d^{5} 2E^{5}$	5/2	$3d^{5} 2n^{5}$	3/2	123.471	118 578				
$3d^{5} 2E^{5}$	5/2	$3d^{5} 2C^{3}$	7/2	75 224	75 182				
$3d^{5}2E^{5}$	5/2	$3d^5 2d^3$	3/2	30 298	20 330				
$3d^{5}2E^{5}$	5/2	$3d^{5} 2D^{1}$	5/2	27 911	27 925				
$3d^{5}2E^{5}$	5/2	$3d^5 4 p^3$	5/2	27.911	27.923				
$3d^{5}2E^{5}$	5/2	$3d^5 4 E^3$	7/2	17 896	17 857				
$3d^{5}2E^{5}$	5/2	$3d^5 4 D^5$	3/2	17.090	17.037				
2452r5	5/2	$2d^{5}2D^{3}$	5/2	17.113	1/.074				
$3d^{5}2E^{5}$	5/2	$3d^{5} 2C^{3}$	7/2	14.949	14.920				
$3d^{5}2E^{5}$	5/2	$3d^{5} 2D^{1}$	3/2	11 250	14.551				
$3d^{5}2E^{5}$	5/2	$3d^{5} 2D^{1}$	5/2	8 4 20	8 403				
3d5 2 Ц3	9/2	$3d^{5} 2c^{5}$	7/2	0.420 486 710	404 2 18				
3d5 2 Ц3	9/2	$3d^{5} 2C^{3}$	7/2	400.710	110 603				
зи II 245 2 ЦЗ	9/2	$2452C^3$	0/2	61 605	61 720				
зи II 245 2 ЦЗ	9/2	2454E3	7/2 7/2	10 267	10 227				
зи П ⁻ 245 2 Ц3	9/2	2452113	11/2	19.307	19.527				
2452113	9/2	2452C5	0/2	16.900	16.003				
2452113	9/2	$3u^{5} - G^{3}$	7/2 7/2	10.902	15 262				
2452C5	7/2	$34^5 4 E^3$	5/2	13.202 508 575	587.600				
$3u^{2} - G^{2}$	7/2	$2452C^3$	7/2	142 074	142 402				
$3u^{2} - G^{2}$	7/2	$345 2C^3$	0/2	70 522	70 552				
$3u^{2} - G^{2}$	7/2	2 d5 2 D1	9/2 5/2	22.865	22.867				
3d5 2C5	7/2	$3d^5 4 D^3$	5/2	23,638	23 555				
3452C5	7/2	345 4 E3	7/2	20.050	20.113				
2452C5	7/2	2452C5	0/2	17 505	17 550				
3u G $2d^{5} 2C^{5}$	7/2	3u G $2d^{5} 2n^{3}$	9/2 5/2	17.595	16 472				
3u G $2d^{5} 2C^{5}$	7/2	$2452C^{3}$	7/2	16.303	15.475				
$3d^{5} 2c^{5}$	7/2	$3d^{5} 2D^{1}$	5/2	8 807	8 871				
$3d^5 4E^3$	5/2	$3d^{5} 2D^{5}$	3/2	2038 287	2231 127				
$3d^5 4 E^3$	5/2	$3d^{5} C^{3}$	7/2	187 841	188 108				
$3d^5 4E^3$	5/2	$3d^5 2p^3$	3/2	39 944	40.038				
$3d^5 4 E^3$	5/2	$3d^{5} 2D^{1}$	5/2	35 896	35 030				
$3d^5 4 E^3$	5/2	$3d^5 4p^3$	5/2	24.610	24 539				
$3d^5 4 E^3$	5/2	$3d^5 4 E^3$	7/2	24.010	24.007				
$3d^5 4 E^3$	5/2	3d ⁵ 4D ⁵	3/2	19 815	10.020				
$3d^5 4 E^3$	5/2	$3d^{5} 2D^{3}$	5/2	19.813	16.048				
$3d^{5}4r^{3}$	5/2	$3d^{5}2^{3}$	7/2	16 205	16 192				
$3d^{5} 4r^{3}$	5/2	3d ⁵ ² n ¹	3/2	12 360	12 356				
$3d^{5} 4r^{3}$	5/2	$3d^{5} 2n^{1}$	5/2	0 0 2 6	9 007				
$3d^{5} 2n^{5}$	3/2	$3d^5 4 p^3$	1/2	205 353	204 122				
$3d^{5} 2n^{5}$	3/2	$3d^{5} 2p^{3}$	1/2 2/2	203.333 40 742	40 770				
$3d^{5} {}^{2} \Pi^{5}$	3/2	$3d^{5} 2n^{1}$	5/2	36 540	36 527				
3d ⁵ ² D ⁵	3/2	$3d^5 4 p^3$	5/2	24 911	24 812				
$3d^{5} {}^{2}D^{5}$	3/2	$3d^{5} {}^{4}D^{5}$	3/2	20.010	19.946				

Table 5. Cont.

Label a	nd J	Label a	nd J	Present	Work	Expt			
for Lo	wer	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ⁵ ² D ⁵	3/2	3d ⁵ ² D ³	5/2	17 114	17 078				
$3d^{5} {}^{2}D^{5}$	3/2	$3d^{5} 2p^{3}$	1/2	14 828	14 805				
$3d^{5} {}^{2}D^{5}$	3/2	$3d^{5} {}^{2}D^{1}$	3/2	12.445	12.425				
$3d^{5} {}^{2}D^{5}$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	9.066	9 044				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}G^{3}$	9/2	139 208	139 747				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	44.377	44.427				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{4}P^{3}$	5/2	28.321	28.220				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{4}F^{3}$	7/2	23.482	23.419				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}G^{5}$	9/2	20.065	20.027				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}D^{3}$	5/2	18.657	18.626				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}G^{3}$	7/2	17.735	17.707				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	9.482	9.460				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}P^{3}$	3/2	50.826	50.945				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{4}D^{5}$	3/2	22.170	22.106				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}P^{3}$	1/2	15.982	15.963				
$3d^{5} {}^{4}P^{3}$	1/2	$3d^{5} {}^{2}D^{1}$	3/2	13.248	13.230				
$3d^{5} {}^{2}G^{3}$	9/2	$3d^{5} {}^{4}F^{3}$	7/2	28.247	28.134				
$3d^{5} {}^{2}G^{3}$	9/2	$3d^{5} {}^{2}H^{3}$	11/2	27.264	27.162				
$3d^{5} {}^{2}G^{3}$	9/2	$3d^{5} {}^{2}G^{5}$	9/2	23.444	23.377				
$3d^{5} {}^{2}G^{3}$	9/2	$3d^{5} {}^{2}G^{3}$	7/2	20.324	20.276				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	354.267	351.029				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{4}P^{3}$	5/2	64.110	63.389				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{4}D^{5}$	3/2	39.323	39.051				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{2}D^{3}$	5/2	29.510	29.388				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{2}P^{3}$	1/2	23.312	23.247				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{2}D^{1}$	3/2	17.918	17.871				
$3d^{5} {}^{2}P^{3}$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	11.661	11.621				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{4}P^{3}$	5/2	78.275	77.359				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{4}F^{3}$	7/2	49.873	49.527				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{4}D^{5}$	3/2	44.232	43.939				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{2}D^{3}$	5/2	32.191	32.073				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{2}G^{3}$	7/2	29.540	29.440				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	18.873	18.830				
$3d^{5} {}^{2}D^{1}$	5/2	$3d^{5} {}^{2}D^{1}$	5/2	12.058	12.019				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^5 {}^4F^3$	7/2	137.450	137.658				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^{5} {}^{4}D^{5}$	3/2	101.706	101.709				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^{5} {}^{2}D^{3}$	5/2	54.677	54.789				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^{5} {}^{2}G^{3}$	7/2	47.445	47.528				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	24.869	24.888				
$3d^{5} {}^{4}P^{3}$	5/2	$3d^{5} {}^{2}D^{1}$	5/2	14.254	14.230				
$3d^{5} {}^{4}F^{3}$	7/2	$3d^{5} {}^{2}G^{5}$	9/2	137.868	138.255				
$3d^{5} {}^{4}F^{3}$	7/2	$3d^{5} {}^{2}D^{3}$	5/2	90.796	91.013				
$3d^{5} {}^{4}F^{3}$	7/2	$3d^{5} = G^{3}$	7/2	72.454	72.591				
$3d^{5} {}^{4}F^{3}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	15.903	15.871				
$3d^{3} = 4H^{3}$	11/2	$3d^{5} = 4G^{5}$	9/2	167.319	167.768				
$3d^{5} = D^{5}$	3/2	$3d^{5} = 2D^{3}$	5/2	118.248	118.767				
$3d^{5} + D^{5}$	3/2	$3d^{5} = 2P^{5}$	1/2	57.255	57.442				
$3d^{3} + D^{3}$	3/2	$3d^{5} = D^{1}$	3/2	32.917	32.951				
$3d^{3} + D^{3}$	3/2	$3d^{5} = D^{1}$	5/2	16.577	16.545				
3d ⁵ 4G ⁵	9/2	$3d^{5/2}G^{3}$	7/2	152.705	152.840				

Table 5. Cont.

Label a	nd J	Label a	nd J	Present	Work	Expt	GRASP	RMBPTg	RCIg
	ver	for Up	per	n = 5	n = 0	(Kei. [2])			
$3d^{5} {}^{2}D^{3}$	5/2	$3d^{5} {}^{2}G^{3}$	7/2	358.662	358.634				
$3d^{5} {}^{2}D^{3}$	5/2	$3d^{5} {}^{2}D^{1}$	3/2	45.616	45.602				
$3d^{5} {}^{2}D^{3}$	5/2	$3d^{5} {}^{2}D^{1}$	5/2	19.280	19.223				
$3d^{5} {}^{2}G^{3}$	7/2	$3d^{5} {}^{2}D^{1}$	5/2	20.376	20.312				
$3d^{5} {}^{2}P^{3}$	1/2	$3d^{5} {}^{2}D^{1}$	3/2	77.440	77.283				
$3d^{5} {}^{2}D^{1}$	3/2	$3d^{5} {}^{2}D^{1}$	5/2	33.396	33.231				
W ⁵⁰⁺ (Cr-	like)								
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{5}D^{4}$	3	19.752	19.720	19.684(3)	19.796	19.693	19.835
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{5}D^{4}$	4	19.291	19.267	19.239(3)	19.303	19.237	19.425
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}G^{4}$	5	17.162	17.150	17.133(3)	17.118	17.131	17.259
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}D^{4}$	3	15.390	15.378	15.363(3)	15.370	15.289	15.316
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{1}G^{2}$	4	13.147	13.139	13.137(3)	13.114	13.153	13.050
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{2}$	3	12.785	12.779	12.779(3)	12.739	12.800	12.642
$3d^{6} {}^{5}D^{4}$	4	3d ^{6 3} H ⁴	4	9.024	9.013				
$3d^{6} {}^{5}D^{4}$	4	3d ^{6 5} D ⁴	3	8.809	8.798				
$3d^{6} {}^{5}D^{4}$	4	3d ^{6 3} H ⁴	5	8.756	8.746				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{4}$	3	8.356	8.347				
3d ^{6 5} D ⁴	4	$3d^{6} {}^{1}G^{4}$	4	8.111	8.104				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{2}$	4	7.274	7.269				
3d ^{6 5} D ⁴	4	$3d^{6} {}^{1}G^{2}$	4	5.668	5.661				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{2}$	3	5.461	5.455				
$3d^{6} {}^{3}D^{4}$	2	3d ^{6 5} D ⁴	3	22.546	22.503				
$3d^{6} {}^{3}D^{4}$	2	3d ^{6 5} D ⁴	1	20.709	20.668				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{4}$	2	17.384	17.367				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}D^{4}$	3	17.035	17.019				
$3d^{6} {}^{3}D^{4}$	2	3d ^{6 3} D ⁴	2	14.214	14.202	14.193(3)	14.184	14.202	14.170
$3d^{6} {}^{3}D^{4}$	2	3d ^{6 3} P ²	1	14.198	14.188				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{2}$	3	13.900	13.892	13.886(3)	13.843	13.895	13.848
$3d^{6} {}^{3}D^{4}$	2	3d ^{6 5} D ⁴	2	10.042	10.025				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{5}D^{4}$	3	9.324	9.312				
3d ⁶ ³ D ⁴	2	3d ^{6 3} F ⁴	3	8.818	8.808				
3d ⁶ ³ D ⁴	2	3d ^{6 3} D ⁴	1	8.662	8.652				
3d ⁶ ³ D ⁴	2	3d ^{6 3} F ⁴	2	8.468	8.460				
3d ^{6 3} D ⁴	2	$3d^{6} {}^{3}F^{2}$	2	7.848	7.839				
3d ^{6 3} D ⁴	2	$3d^{6} {}^{1}D^{2}$	2	6.867	6.863				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	1	6.248	6.238				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	2	5.711	5.704				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{2}$	3	5.655	5.648				
$3d^{6} {}^{3}P^{2}$	0	$3d^{6} {}^{5}D^{4}$	1	29.559	29.509				
$3d^{6} {}^{3}P^{2}$	0	$3d^{6} {}^{3}P^{2}$	1	17.865	17.861	17.826(3)	17.750	17.837	17.921
$3d^{6} {}^{3}P^{2}$	0	$3d^{6} {}^{3}D^{4}$	1	9.901	9.893				
$3d^{6} {}^{3}P^{2}$	0	$3d^{6} {}^{3}P^{2}$	1	6.868	6.858				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{5}D^{4}$	4	827.797	838.107				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}F^{4}$	2	75.926	76.090				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}D^{4}$	3	69.700	69.830				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} G^{2}$	4	39.314	39.365				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}D^{4}$	2	38.467	38.499				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}F^{2}$	3	36.246	36.304				
3d ^{6 5} D ⁴	3	3d ^{6 5} D ⁴	2	18.107	18.080				

Table 5. Cont.

Label and <i>I</i>		Label and I		Present Work		Expt			
for Lowe	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ^{6 5} D ⁴	3	3d ^{6 3} H ⁴	4	16 615	16 599				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{5}D^{4}$	3	15.900	15.886				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}F^{4}$	3	14.482	14.472				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{1}G^{4}$	4	13 764	13 758				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}F^{4}$	2	13 562	13,556				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} 3F^{2}$	2	12.038	12 029				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}F^{2}$	4	11 514	11.512				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{1}D^{2}$	2	9 875	9 874				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{1}G^{2}$	4	7 949	7 940				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}P^{2}$	2	7.648	7.641				
$3d^{6} {}^{5}D^{4}$	3	$3d^{6} {}^{3}F^{2}$	3	7.547	7.540				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}G^{4}$	5	155.438	156.080				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}D^{4}$	3	76.108	76.177				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{1}G^{2}$	4	41.274	41.305				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{2}$	3	37.905	37.948				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}H^{4}$	4	16.955	16.934				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{5}D^{4}$	3	16.211	16.193				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}H^{4}$	5	16.032	16.018				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{4}$	3	14.740	14.726				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{1}G^{4}$	4	13.997	13.987				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{2}$	4	11.676	11.672				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{1}G^{2}$	4	8.026	8.016				
$3d^{6} {}^{5}D^{4}$	4	$3d^{6} {}^{3}F^{2}$	3	7.617	7.609				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}F^{4}$	2	108.263	108.730				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}P^{4}$	0	55.744	55.924				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}D^{4}$	2	45.325	45.393				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	1	45.157	45.248				
$3d^{6} {}^{5}D^{4}$	1	3d ^{6 5} D ⁴	2	19.495	19.468				
$3d^{6} {}^{5}D^{4}$	1	3d ^{6 5} D ⁴	0	18.606	18.576				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}D^{4}$	1	14.889	14.882				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}F^{4}$	2	14.326	14.322				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}F^{2}$	2	12.637	12.629				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{1}D^{2}$	2	10.274	10.274				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{1}S^{0}$	0	8.969	8.968				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	1	8.947	8.934				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	2	7.886	7.878				
$3d^{6} {}^{5}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	0	5.630	5.622				
$3d^{6} {}^{3}H^{4}$	6	$3d^{6} {}^{3}G^{4}$	5	33171.897	25414.252				
$3d^{6} {}^{3}H^{4}$	6	$3d^{6} {}^{3}H^{4}$	5	17.866	17.837				
$3d^{6} {}^{3}H^{4}$	6	$3d^{6\ 1}I^4$	6	17.042	17.020				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6} {}^{1}G^{2}$	4	56.196	56.170				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6} {}^{3}H^{4}$	4	19.031	18.995				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6} {}^{3}H^{4}$	5	17.876	17.850				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6\ 1}I^4$	6	17.051	17.032				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6} {}^{1}G^{4}$	4	15.382	15.364				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6} {}^{3}F^{2}$	4	12.625	12.615				
$3d^{6} {}^{3}G^{4}$	5	$3d^{6} {}^{1}G^{2}$	4	8.463	8.450				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}D^{4}$	3	850.017	848.731				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}D^{4}$	2	77.967	77.927				
$3d^{6} {}^{3}F^{4}$	2	3d ^{6 3} P ²	1	77.469	77.499				

Table 5. Cont.

Label and J		Label and J		Present Work		Expt	CDACD		
for Lowe	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GKASP	KMBPIg	кСІg
3d ⁶ ³ F ⁴	2	$3d^{6} {}^{3}F^{2}$	3	69.354	69.431				
$3d^{6} {}^{3}F^{4}$	2	3d ^{6 5} D ⁴	2	23.777	23.715				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{5}D^{4}$	3	20.111	20.078				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}F^{4}$	3	17.895	17.871				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}D^{4}$	1	17.263	17.242				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}F^{4}$	2	16.511	16.494				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}F^{2}$	2	14.307	14.288				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{1}D^{2}$	2	11.351	11.346				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}P^{2}$	1	9.754	9.734				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}P^{2}$	2	8.505	8.494				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}F^{2}$	3	8.381	8.370				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{1}G^{2}$	4	90.179	90.232				
3d ⁶ ³ D ⁴	3	$3d^{6} {}^{3}D^{4}$	2	85.841	85.805				
3d ⁶ ³ D ⁴	3	$3d^{6} {}^{3}F^{2}$	3	75.516	75.617				
3d ⁶ ³ D ⁴	3	$3d^{6} {}^{5}D^{4}$	2	24.461	24.396				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{3}H^{4}$	4	21.815	21.774				
3d ⁶ ³ D ⁴	3	$3d^{6} {}^{5}D^{4}$	3	20.598	20.565				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{3}F^{4}$	3	18.280	18.255				
3d ⁶ ³ D ⁴	3	$3d^{6} {}^{1}G^{4}$	4	17.151	17.133				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{3}F^{4}$	2	16.838	16.821				
3d ⁶ ³ D ⁴	3	$3d^{6} {}^{3}F^{2}$	2	14.552	14.533				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{3}F^{2}$	4	13.792	13.784				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{1}D^{2}$	2	11.505	11.500				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{1}G^{2}$	4	8.972	8.959				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{3}P^{2}$	2	8.591	8.579				
$3d^{6} {}^{3}D^{4}$	3	$3d^{6} {}^{3}F^{2}$	3	8.464	8.453				
$3d^{6} {}^{3}P^{4}$	0	$3d^{6} {}^{3}P^{2}$	1	237.757	237.023				
$3d^{6} {}^{3}P^{4}$	0	$3d^{6} {}^{3}D^{4}$	1	20.315	20.278				
$3d^{6} {}^{3}P^{4}$	0	$3d^{6} {}^{3}P^{2}$	1	10.658	10.633				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{3}F^{2}$	3	464.412	466.858				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{3}H^{4}$	4	28.776	28.700				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{5}D^{4}$	3	26.696	26.635				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{3}H^{4}$	5	26.215	26.164				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{3}F^{4}$	3	22.928	22.886				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{1}G^{4}$	4	21.178	21.149				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{3}F^{2}$	4	16.283	16.269				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{1}G^{2}$	4	9.963	9.946				
$3d^{6} {}^{1}G^{2}$	4	$3d^{6} {}^{3}F^{2}$	3	9.341	9.327				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	1	12130.770	14130.082				
3d ⁶ ³ D ⁴	2	$3d^{6} {}^{3}F^{2}$	3	627.813	636.845				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{5}D^{4}$	2	34.209	34.088				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{5}D^{4}$	3	27.101	27.047				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{4}$	3	23.226	23.189				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}D^{4}$	1	22.172	22.140				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{4}$	2	20.946	20.922				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{2}$	2	17.522	17.497				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{1}D^{2}$	2	13.285	13.280				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	1	11.148	11.124				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	2	9.546	9.533				
$3d^{6} {}^{3}D^{4}$	2	$3d^{6} {}^{3}F^{2}$	3	9.390	9.377				

Table 5. Cont.

Label and <i>I</i>		Label and I		Present Work		Expt			
for Lowe	er	for Upp	er	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d6 3 p2	1	3,765,04	2	34 306	34 171				
$3d^{6} 3p^{2}$	1	$3d^{6} {}^{5}D^{4}$	0	31.646	31 512				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}D^{4}$	1	22.213	22.175				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}F^{4}$	2	20.982	20.954				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}F^{2}$	2	17.548	17.518				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{1}D^{2}$	2	13.300	13.292				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{1}S^{0}$	0	11.192	11.185				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}P^{2}$	1	11.158	11.132				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}P^{2}$	2	9.554	9.539				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}P^{2}$	0	6.432	6.419				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{5}D^{4}$	2	36.181	36.016				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}H^{4}$	4	30.677	30.580				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{5}D^{4}$	3	28.324	28.246				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}F^{4}$	3	24.119	24.065				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{1}G^{4}$	4	22.190	22.153				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}F^{4}$	2	21.669	21.633				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}F^{2}$	2	18.025	17.991				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}F^{2}$	4	16.875	16.857				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{1}D^{2}$	2	13.572	13.563				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{1}G^{2}$	4	10.182	10.163				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}P^{2}$	2	9.694	9.677				
$3d^{6} {}^{3}F^{2}$	3	$3d^{6} {}^{3}F^{2}$	3	9.532	9.517				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{5}D^{4}$	3	130.436	130.930				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}F^{4}$	3	72.345	72.524				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}D^{4}$	1	63.013	63.168				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}F^{4}$	2	54.026	54.171				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}F^{2}$	2	35.921	35.947				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{1}D^{2}$	2	21.720	21.755				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	1	16.537	16.511				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}P^{2}$	2	13.242	13.233				
$3d^{6} {}^{5}D^{4}$	2	$3d^{6} {}^{3}F^{2}$	3	12.942	12.935				
$3d^{6} {}^{5}D^{4}$	0	$3d^{6} {}^{3}D^{4}$	1	74.520	74.840				
$3d^{6} {}^{5}D^{4}$	0	$3d^{6} {}^{3}P^{2}$	1	17.236	17.213				
$3d^{6} {}^{3}H^{4}$	4	$3d^{6} {}^{5}D^{4}$	3	369.368	370.105				
$3d^{6}{}^{3}H^{4}$	4	$3d^{6} {}^{3}H^{4}$	5	294.589	296.075				
$3d^{6}{}^{3}H^{4}$	4	$3d^{\circ 5}F^{4}$	3	112.825	112.959				
$3d^{6}{}^{3}H^{4}$	4	$3d^{6-1}G^{4}$	4	80.216	80.382				
$3d^{6}{}^{3}H^{4}$	4	$3d^{6}{}^{5}F^{2}$	4	37.506	37.563				
$3d^{6}{}^{5}H^{4}$	4	$3d^{6-1}G^{2}$	4	15.240	15.221				
$3d^{6}{}^{5}H^{4}$	4	$3d^{6} {}^{5}F^{2}$	3	13.830	13.817				
$3d^{6} {}^{5}D^{4}$	3	$3d^{0} F^{4}$	3	162.444	162.579				
3a~ ~D ⁺ 246.5 D4	3	3a~ 1G1 2 46 3 F4	4	102.469	102.683				
346 5 D ⁴	3	30° ° F 1 2 46 3 F2	2	92.227 40 574	92.402 40 552				
246 5 D4	3	2463r2	۲ ۸	49.3/4	47.002 41.905				
346 5 D-	3 2	346 1 m2	4 ว	41.744 26.050	41.000 26.000				
3d ⁶ ⁵ D ⁴	3 2	3d61C2	∠ 1	20.009	20.090 15.974				
3d ^{6 5} D ⁴	3	3d6 3 D2	+)	14 738	10.074				
3d ⁶ ⁵ D ⁴	3	3d6 3 E2	∠ 3	14 368	14 353				
$3d^{6} {}^{3}H^{4}$	5	$3d^{6} {}^{1}I^{4}$	6	369.318	371.637				

Table 5. Cont.

Label and J		Label and J		Present Work		Expt			
for Lov	ver	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ⁶ ³ H ⁴	5	$3d^{6} {}^{1}G^{4}$	4	110.232	110.337				
$3d^{6} {}^{3}H^{4}$	5	$3d^{6} {}^{3}F^{2}$	4	42.977	43.021				
$3d^{6} {}^{3}H^{4}$	5	$3d^{6} {}^{1}G^{2}$	4	16.071	16.046				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{1}G^{4}$	4	277.541	278.717				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{3}F^{4}$	2	213.361	214.066				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{3}F^{2}$	2	71.346	71.275				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{3}F^{2}$	4	56.181	56.276				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{1}D^{2}$	2	31.039	31.076				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{1}G^{2}$	4	17.620	17.592				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{3}P^{2}$	2	16.208	16.187				
$3d^{6} {}^{3}F^{4}$	3	$3d^{6} {}^{3}F^{2}$	3	15.762	15.743				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{3}F^{4}$	2	378.830	380.349				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{3}F^{2}$	2	83.550	83.418				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{1}D^{2}$	2	33.145	33.182				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{1}S^{0}$	0	22.557	22.569				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	1	22.422	22.355				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	2	16.764	16.740				
$3d^{6} {}^{3}D^{4}$	1	$3d^{6} {}^{3}P^{2}$	0	9.053	9.035				
$3d^{6} {}^{1}G^{4}$	4	$3d^{6} {}^{3}F^{2}$	4	70.440	70.514				
$3d^{6} {}^{1}G^{4}$	4	$3d^{6} {}^{1}G^{2}$	4	18.815	18.777				
$3d^{6} {}^{1}G^{4}$	4	$3d^{6} {}^{3}F^{2}$	3	16.711	16.685				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}F^{2}$	2	107.190	106.853				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{1}D^{2}$	2	36.323	36.354				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}P^{2}$	1	23.832	23.751				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}P^{2}$	2	17.541	17.511				
$3d^{6} {}^{3}F^{4}$	2	$3d^{6} {}^{3}F^{2}$	3	17.019	16.992				
$3d^{6} {}^{3}F^{2}$	2	$3d^{6} {}^{1}D^{2}$	2	54.939	55.101				
$3d^{6} {}^{3}F^{2}$	2	$3d^{6} {}^{3}P^{2}$	1	30.646	30.539				
$3d^{6} {}^{3}F^{2}$	2	$3d^{6} {}^{3}P^{2}$	2	20.973	20.943				
$3d^{6} {}^{3}F^{2}$	2	$3d^{6} {}^{3}F^{2}$	3	20.232	20.205				
$3d^{6} {}^{3}F^{2}$	4	$3d^{6} {}^{1}G^{2}$	4	25.671	25.592				
$3d^{6} {}^{3}F^{2}$	4	$3d^{6} {}^{3}F^{2}$	3	21.909	21.857				
$3d^{6} {}^{1}D^{2}$	2	$3d^{6} {}^{3}P^{2}$	1	69.307	68.508				
$3d^{6} {}^{1}D^{2}$	2	$3d^{6} {}^{3}P^{2}$	2	33.922	33.783				
$3d^{6} {}^{1}D^{2}$	2	$3d^{6} {}^{3}F^{2}$	3	32.025	31.905				
$3d^{6} {}^{1}S^{0}$	0	$3d^{6} {}^{3}P^{2}$	1	3732.652	2353.561				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}P^{2}$	2	66.443	66.648				
$3d^{6} {}^{3}P^{2}$	1	$3d^{6} {}^{3}P^{2}$	0	15.184	15.162				
$3d^{6} {}^{1}G^{2}$	4	3d ^{6 3} F ²	3	149.470	149.753				
3d ^{6 3} P ²	2	$3d^{6} {}^{3}F^{2}$	3	572.500	573.976				
W ⁴⁹⁺ (Mr	n-like)								
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{4}F^{3}$	7/2	18.940	18.908	18.880(3)	19.006	18.901	18.943
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{4}F^{3}$	9/2	17.138	17.119	17.106(3)	17.149	17.118	17.132
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{2}H^{3}$	11/2	15.381	15.371	15.368(3)	15.343	15.372	15.380
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{2}F^{3}$	7/2	14.180	14.170	14.166(3)	14.156	14.187	14.063
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{2}H^{3}$	9/2	8.434	8.424				
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{2}F^{3}$	7/2	8.259	8.250				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	5/2	174.708	174.056				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{4}P^{3}$	3/2	19.753	19.715				

Table 5. Cont.

Label and J		Label and J		Present Work		Expt	00400		
for Lov	ver	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	RMBPT _g	RCIg
3d ⁷ ² P ³	3/2	$3d^{7} {}^{4}P^{3}$	5/2	19.111	19.081	19.047(3)	19.130	19.037	19.271
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{4}P^{3}$	1/2	18.720	18.692	18.670(3)	18.764	18.680	18.733
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{2}F^{3}$	5/2	15.597	15.585				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	3/2	12.711	12.700				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{4}F^{3}$	5/2	9.864	9.847				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{4}P^{3}$	3/2	9.561	9.546				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{2}P^{3}$	1/2	9.171	9.157				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	5/2	7.643	7.636				
$3d^{7} {}^{2}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	3/2	6.060	6.050				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{4}F^{3}$	7/2	27.098	27.043				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{4}P^{3}$	3/2	22.271	22.233				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{4}P^{3}$	5/2	21.458	21.430				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}F^{3}$	7/2	18.307	18.294	18.276(3)	18.258	18.274	18.425
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}F^{3}$	5/2	17.126	17.117				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	13.709	13.700				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{4}F^{3}$	5/2	10.455	10.437				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{4}P^{3}$	3/2	10.115	10.099				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}F^{3}$	7/2	9.507	9.496				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}D^{1}$	5/2	7.993	7.986				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	6.278	6.268				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{4}F^{3}$	9/2	180.107	180.908				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{4}P^{3}$	5/2	103.103	103.259				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{2}F^{3}$	7/2	56.428	56.550				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{2}F^{3}$	5/2	46.537	46.637				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{4}F^{3}$	5/2	17.022	16.998				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{2}H^{3}$	9/2	15.204	15.193				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{2}F^{3}$	7/2	14.645	14.635				
$3d^{7} {}^{4}F^{3}$	7/2	$3d^{7} {}^{2}D^{1}$	5/2	11.337	11.332				
$3d^{7} {}^{4}F^{3}$	9/2	3d ^{7 2} H ³	11/2	150.021	150.559				
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{2}F^{3}$	7/2	82.173	82.265				
$3d^{7} {}^{4}F^{3}$	9/2	3d ^{7 2} H ³	9/2	16.606	16.586				
$3d^{7} {}^{4}F^{3}$	9/2	$3d^{7} {}^{2}F^{3}$	7/2	15.942	15.923				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{4}P^{3}$	5/2	587.816	593.270				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{4}P^{3}$	1/2	357.969	360.283				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}F^{3}$	5/2	74.127	74.387				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	3/2	35.657	35.693				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{4}F^{3}$	5/2	19.704	19.673				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{4}P^{3}$	3/2	18.530	18.506				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}P^{3}$	1/2	17.118	17.100				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	5/2	12.467	12.462				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	3/2	8.742	8.729				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7} {}^{2}F^{3}$	7/2	124.648	125.014				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7} {}^{2}F^{3}$	5/2	84.823	85.051				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	37.960	37.978				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^7 {}^4F^3$	5/2	20.388	20.347				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7} {}^{4}P^{3}$	3/2	19.133	19.101				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7/2}F^{3}$	7/2	17.070	17.052				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7/2}D^1$	5/2	12.737	12.729				
$3d^{7} {}^{4}P^{3}$	5/2	$3d^{7/2}D^{1}$	3/2	8.874	8.860				
$3d^{7} {}^{4}P^{3}$	1/2	$3d^{7/2}D^{1}$	3/2	39.602	39.618				

Table 5. Cont.

Label and J		Label and J		Present Work		Expt	CDACD	Д МДРТ	
for Lo	wer	for Up	per	n = 5	n = 6	(Ref. [2])	GRASP	KMBP1g	кСІ _g
3d ⁷ ⁴ P ³	1/2	$3d^{7} {}^{4}P^{3}$	3/2	19.542	19.508				
$3d^{7} {}^{4}P^{3}$	1/2	$3d^{7} {}^{2}P^{3}$	1/2	17.978	17.952				
$3d^{7} {}^{4}P^{3}$	1/2	$3d^{7} {}^{2}D^{1}$	3/2	8.961	8.946				
3d ^{7 2} H ³	11/2	$3d^{7} {}^{2}H^{3}$	9/2	18.673	18.639				
$3d^{7} {}^{2}F^{3}$	7/2	$3d^{7} {}^{2}F^{3}$	5/2	265.490	266.061				
$3d^{7} {}^{2}F^{3}$	7/2	$3d^{7} {}^{4}F^{3}$	5/2	24.375	24.303				
$3d^{7} {}^{2}F^{3}$	7/2	$3d^{7} {}^{2}H^{3}$	9/2	20.812	20.774				
$3d^{7} {}^{2}F^{3}$	7/2	$3d^{7} {}^{2}F^{3}$	7/2	19.779	19.745				
$3d^{7} {}^{2}F^{3}$	7/2	$3d^{7} {}^{2}D^{1}$	5/2	14.187	14.173				
$3d^{7} {}^{2}F^{3}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	68.707	68.619				
$3d^{7} {}^{2}F^{3}$	5/2	$3d^{7} {}^{4}F^{3}$	5/2	26.839	26.746				
$3d^{7} {}^{2}F^{3}$	5/2	$3d^{7} {}^{4}P^{3}$	3/2	24.706	24.634				
$3d^{7} {}^{2}F^{3}$	5/2	$3d^{7} {}^{2}F^{3}$	7/2	21.371	21.328				
$3d^{7} {}^{2}F^{3}$	5/2	$3d^{7} {}^{2}D^{1}$	5/2	14.988	14.970				
$3d^{7} {}^{2}F^{3}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	9.911	9.890				
$3d^{7} {}^{2}D^{1}$	3/2	$3d^{7} {}^{4}F^{3}$	5/2	44.043	43.830				
$3d^{7} {}^{2}D^{1}$	3/2	$3d^{7} {}^{4}P^{3}$	3/2	38.579	38.430				
$3d^{7} {}^{2}D^{1}$	3/2	$3d^{7} {}^{2}P^{3}$	1/2	32.925	32.828				
$3d^{7} {}^{2}D^{1}$	3/2	$3d^{7} {}^{2}D^{1}$	5/2	19.169	19.147				
$3d^{7} {}^{2}D^{1}$	3/2	$3d^{7} {}^{2}D^{1}$	3/2	11.581	11.555				
$3d^{7} {}^{4}F^{3}$	5/2	$3d^{7} {}^{4}P^{3}$	3/2	310.962	311.919				
$3d^{7} {}^{4}F^{3}$	5/2	$3d^{7} {}^{2}F^{3}$	7/2	104.893	105.290				
$3d^{7} {}^{4}F^{3}$	5/2	$3d^{7} {}^{2}D^{1}$	5/2	33.943	34.000				
$3d^{7} {}^{4}F^{3}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	15.713	15.692				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}P^{3}$	1/2	224.661	225.205				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	5/2	38.102	38.159				
$3d^{7} {}^{4}P^{3}$	3/2	$3d^{7} {}^{2}D^{1}$	3/2	16.549	16.524				
$3d^{7} {}^{2}P^{3}$	1/2	$3d^{7} {}^{2}D^{1}$	3/2	17.865	17.832				
$3d^{7} {}^{2}H^{3}$	9/2	$3d^{7} {}^{2}F^{3}$	7/2	398.243	398.611				
$3d^{7} {}^{2}F^{3}$	7/2	$3d^{7} {}^{2}D^{1}$	5/2	50.182	50.215				
$3d^{7} {}^{2}D^{1}$	5/2	$3d^{7} {}^{2}D^{1}$	3/2	29.257	29.143				
W ⁴⁸⁺ (Fe	-like)								
- 18 3 F	11111	0.18.3 E		10.041	10.000	10.000/2)	10.11.1	10.007	10.007
$3d^{6-5}F$	4	$3d^{6} {}^{5}F$	3	19.041	19.009	18.988(3)	19.114	19.007	19.027
$3d^{6} {}^{5}F$	4	$3d^{6-1}G$	4	15.531	15.518	15.511(3)	15.503	15.463	15.525
$3d^{0-1}D$	2	$3d^{6}$ ³ F	3	22.073	22.029	10.050(0)	10.050	10,000	10.044
$3d^{0-1}D$	2	$3d^{6} {}^{5}P$	2	18.931	18.902	18.878(3)	18.978	18.888	18.966
$3d^{6-1}D$	2	3 <i>a</i> ^{o s} P	1	17.548	17.525	17.502(3)	17.548	17.517	17.489
$3d^{6-1}D$	2	$3a^{\circ 5}F$	2	9.664	9.648				
$3d^{6} {}^{5}P$	0	$3d^{6} {}^{5}P$	1	24.268	24.236				
30° ³ F	3	$3a^{\circ} {}^{\circ}P$	2	132.993	133.189				
30° ³ F	3	$3a^{\circ} G$	4	84.240	84.489				
$3a^{\circ 3}F$	3	$3a^{\circ}$ F	2	17.190	17.167				
$3d^{\circ 3}P$	2	$3d^{\circ} {}^{\circ}P$	1	240.207	240.600				
$3d^{\circ 3}P$	2	$3d^{\circ 3}F$	2	19.742	19.707				
$3d^{\circ 3}P$	1	$3d^{\circ 3}F$	2	21.510	21.465				
3d° ³ P	1	3d° 1S	0	15.102	15.082				
W ⁴⁷⁺ (Co	-like)								
$3d^{9} {}^{2}D$	5/2	3d ⁹ ² D	3/2	18.615	18.586	18.567(3)	18.671	18.586	18.580

Table 5. Cont.

4. Conclusions

The present study has shown that the inclusion of core correlation effects improves the accuracy of theoretical transition wavelengths for M1 transitions in $3d^k$ configurations of tungsten ions. Omitted in our work were correlation effects arising from the $1s^2$ core. Further studies are needed to determine whether the discrepancy with observation arises from the limited orbital set for core correlation or from the inactive $1s^2$ shell in our present work.

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