Second spectrum of Chromium (Cr II) Part I: New energy level reanalysis

Safa Bouazza [a,*], Pascal Quinet [b,c], Patrick Palmeri [b]

[a] *Département de Physique, Université de Reims-Champagne, UFR SEN, BP 1039 F-51687 Reims Cedex 2, France*
[b] *Physique Atomique et Astrophysique, Université de Mons UMONS, B-7000 Mons, Belgium*
[c] *IPNAS, Université de Liège, B-4000 Liège, Belgium*

ARTICLE INFO

ABSTRACT

Using a linked-parametric technique of level-fitting calculations in a multiconfiguration basis, a parametric fine structure (fs) analysis for both even and odd parities of Cr II was achieved. For the first time the fs parameter, magnetic Landé g-factor and the percentage of leading eigenvector values for more than one thousand levels are determined and given for these two sets. This study has led us to confirm in the whole the well founded basis of NIST team works but inevitably also to exchange assignments of some levels classified in earlier lists of energy levels and to shift positions of some quartets like ^4F_J for instance. Furthermore we take this opportunity to add our predicted doublet, quartet and sextet locations for missing experimental levels up to 124,000 cm^{-1}.

Contents

1. Introduction

Chromium is the first element in group 6, of the transition metals, well known for its remarkable magnetic properties: it is the only elemental solid which shows antiferromagnetic ordering at room temperature and below; above 38 °C it changes to paramagnetic. Naturally occurring chromium is composed of three stable isotopes: ^{52}Cr, ^{53}Cr and ^{54}Cr, with abundances of 83.79%, 9.50% and 2.37% and nuclear spins of 0, 3/2 and 0, respectively. Consequentially hyperfine structure (hfs) splitting of only enriched ^{53}Cr exists and was possible to evaluate like in [1,2] for atomic chromium but unfortunately no similar observations were achieved for ionic chromium. Furthermore, up to now, no isotope shift measurements are found in literature. As in many cases for different elements, Kiess [3] initiated the Cr II spectrum analysis. He reported observations of spectra excited in direct current arcs and condensed sparks between chromium electrodes. He succeeded in classifying of 1843 lines linking 138 even-parity levels of $3d^5$, $3d^44s$ and $3d^34s^2$ configurations with 139 odd-parity levels belonging to only one configuration: $3d^44p$. In 1952 Moore published a compilation of the energy levels and some of its ions [4]. This work was updated by Sugar and Corliss in 1985 [5]. Johansson extended the Kiess study a half century later, particularly in the near-infrared region and analyzed 450 additional levels [6]. Sansonetti et al. [7,8] reported in turn new observations of Cr II some years later, in the near-ultra-violet region 1140–3400 Å, using 10.7 m normal incidence vacuum spectrograph and FT700 vacuum ultraviolet Fourier transform spectrometer and then more than 3600 lines were classified linking 283 even levels and 368 odd levels. This work was extended two years later [8] by a large number of measurements in the region 2850–37,900 Å, presenting a list of more than 5300 lines linking this time 456 even and 457 odd levels. In this laborious compilation one can find highly excited level positions of the $3d^45g$, $3d^46g$ and even $3d^46h$ configurations, up to 124,500 cm^{-1}. Finally, let us point also the useful implication in this item of Saloman who gave a general survey of the situation [9].

The aim of this study is to perform oscillator strength parameterization and Hartree–Fock eigenvector calculations. In this regard, it is well known that the use of optimized eigenvectors obtained through a least-squares fitting of the calculated energy levels to the available experimental data may considerably improve the final results, not only for the atomic structure but also for radiative transition rates, magnetic Landé g-factors etc. Moreover,

in many of our previous works, semi-empirically optimized eigenvectors turned out very useful for the confirmation of, or identification of errors in, tentative energy-level analyses. It also helped, on the one hand, in ascertaining the proper spectroscopic designation for identifying experimentally measured but not classified levels and, on the other hand, in predicting energy values of missing (not experimentally observed) levels. We want to take advantage of these excellent works of the NIST team to get level eigenvectors in order to transform into actual intermediate coupling the transition matrix beforehand obtained in pure LS coupling with help of Racah algebra [10–12]. In order to determine the radiative transition rates in the near future, we first need to deeply investigate both odd- and even-parities, i.e. two sets of six and eleven configurations respectively in this work, some of whose of their energy levels are determined experimentally. As severe tests for level eigenvector validity one can use generally experimental hfs data. In the absence of the latter in the case of Cr II we will turn our efforts towards experimental oscillator strength or transition probability values, plentifully available in literature [13–16].

2. Analysis procedure of the fine structure and results

2.1. Even-parity configurations

We gave in our previous papers all details of the analysis procedure used to study fine structure of atoms and ions, see for instance [17–21]. Nevertheless we prefer to remind the reader that this procedure includes electrostatic and spin dependent interactions, which are represented by the Slater integrals F^k, G^k, R^k and the spin–orbit parameters ζ_{nl}. In our model, the configuration interaction was considered among the following even-parity configurations:

$$3d^5 + \sum_{n=4}^{n=9} 3d^4ns + \sum_{n'=4}^{n'=6} 3d^4n'd + 3d^34s^2.$$

The interaction effects with distant configurations influencing the term structure were taken into account by two body parameters α and β representing the one- and two-electron excitations respectively and by the three body parameters $T(d^2s)$, $T2(22)$ and $T3(42)$. The effects of excitations of one electron from a closed shell to an open one were taken into account by electrostatically correlated spin–orbit interaction [22,23]. The other details of the whole procedure used here are described also in Refs. [24–26]. The fs least squares fitting procedure has been carried out over

276 energy levels attributed to this extended model. With 445 parameters, 31 of which being treated as free, a very good fit has been achieved, resulting in a mean deviation for the energy level values of $\sigma(E) = 57$ cm^{-1}. In Table 1 are given the observed energy levels, calculated eigenvalues, percentages of first and second components of the wave functions and their corresponding LS term designations. Moreover in this Table the calculated Landé g_J-factors, deduced from the eigenvector compositions, are compared with experimental ones when they are available in the literature. Tables 2 and 3 contain the values of fs parameters obtained through our fitting procedure. We have mentioned the number of experimental works in the Introduction as large even if many observed energy levels are missing. This is due mainly to the hard and long perusal and careful interpretation of recorded spectra obtained with the help of Fourier Transform spectrometer. For this reason we propose our predicted values in the column 3 of Table 2 to suggest the positions of missing energy levels absent in column 2 with rather quite acceptable accuracy. In this work we have discarded or shifted some questionable energy levels, particularly those concerning 3d^{4}5d ^{4}F. We suggest clarifying the situation of these quartets 3d^{4}5d ^{4}F since from our analysis these levels should be located around proposed values given in Table 4 within uncertainty interval of about 50 cm^{-1}. We have to point out also other divergences with literature data about 3d^4(^{5}D)5d $^6S_{5/2}$ and 3d^4(^{5}D)6d $^6S_{5/2}$. We propose 111,469 cm^{-1} and 119,789 cm^{-1} respectively instead of 109394.430 cm^{-1} and 117672.453 cm^{-1}. In Table 2 we also give our predicted values up to 124000 cm^{-1} in some cases, value close enough to ionization energy: 132971.02 (0.12) cm^{-1} [27]. In general one can observe a satisfactory agreement between the experimental values given in literature and our calculated data. In [27], Sansonetti et al. corrected some assignments proposed two years earlier [8] (some quartets belong rather to 3d^{4}4d than to 3d^{4}5d for instance) and we confirm these changes. Furthermore we agree totally with the optimized energy levels given in Table 3 of [27]. Nevertheless in the energy interval 103,000–108,000 cm^{-1} Sansonetti et al. [27] list the positions for 3d^4(^{3}F)d^{4}F, 3d^4(^{3}P)4d^{4}F and 3d^4(^{3}H)4d^{4}F levels while Saloman [9] preferred to omit these level positions. We have found courageous that Sansonetti provided these questionable data since we think these levels belong really to 3d^{4}4d but there remain sometimes some issues in the level labeling.

2.2. Odd-parity configurations

From our experience in fs studies we know that the investigations of odd-parity configuration levels in neutral and lowly ionized iron-group atoms are more difficult than those concerning even-parity configuration ones due to the presence of complex configuration-interaction effects particularly between configurations of the type 3d^{k}4p, 3d^{k-1}4s4p and 3d^{k-2}4s^{2}4p. In the case of the Cr II spectrum, the levels of 3d^{3}4s4p overlap levels from both the 3d^{2}4s^{2}4p and 3d^{4}4p configurations and generally this entanglement is hard to delimit. In this analysis we have considered only configurations whose experimental energy levels are given in literature, namely:

$$3d^44p + 3d^45p + 3d^46p + 3d^34s4p + 3d^44f + 3d^45f$$

in order to avoid a kind of absorption of fs parameters in the presence of level resonance like electrostatic repulsions for instance. The quasi-totality of experimentally known odd-parity levels, located up to 124,000 cm^{-1}, i.e. 354 levels, were fitted using 23 variable parameters among a total number of 245. Since we have found some wrong experimental levels belonging to the even-parity configurations we first have paid attention to looking for questionable experimental odd-parity levels. For this purpose we have discarded at the beginning the level 3d^3(^{4}F)4s4p(^{1}P)$^4F_{9/2}$ at

105203.460 cm^{-1} because its fitting was very bad. The levels of this quartet might be located higher. In [8] Sansonetti et al. have omitted to list 5 levels of the sextet 3d^4(^{5}D)5p ^{6}F, giving only the level $^6F_{3/2}$. Yet these levels, given previously in [7] exist. In Table 5 we give our fitting procedure results with the calculated g_J-value and leading eigenvector components and in Tables 6–7 are displayed the fs radial parameter values.

3. Conclusion

We took advantage of these huge and excellent works of the NIST team, giving a relevant number of experimental energy levels (more than 500) of the second spectrum of chromium to make a list of at least 1000 Cr II energy levels with high reliability, predicting more than 500 of them, missing in previous works. It is a pity that a Zeeman study was not achieved in the same way because sometimes we have faced some problems and experimental Landé-factors would surely help us to take reasonable decisions, recurring to a comparison with our calculated g_J values. Despite this deficiency we have performed successful fitting procedures with low standard deviations and then without these fingerprints we remain optimistic concerning our computed data and our change proposals too. We will confirm the contributions of this fruitful study in Part II, Part III and Part IV of this global work on the Cr II spectrum, showing very satisfactory agreements between experimental oscillator strengths and our calculated data obtained thanks to our deduced level eigenvector amplitudes, strengthening by the way the well founded basis of our fine structure analysis.

References

[1] T. Reinhardt, J. Maichel, M. Bauman, J. Krüger, Z. Phys. D 34 (1995) 87.
[2] J. Marek, Astron. Astrophys. 44 (1975) 69.
[3] C.C. Kiess, J. Res. Natl. Bur. Stand. 47 (1951) 387.
[4] C.E. Moore, Atomic Energy Levels, Vol. II, National Bureau of Standards, (US), Circular N 467, Washigton DC, 1952.
[5] J. Sugar, C. Corliss, J. Phys. Chem. Ref. Data 14 (Suppl. 2) (1985) 279.
[6] S. Johansson, T. Zethson, H. Hartman, et al., Astron. Astrophys. 361 (2000) 977.
[7] C.J. Sansonetti, F. Kerber, J. Reader, M.R. Rosa, Astrophys. J. Suppl. 153 (2004) 555.
[8] C.J. Sansonetti, G. Nave, J. Reader, F. Kerber, Astrophys. J. Suppl. Ser. 202 (2012) 15.
[9] E.B. Saloman, J. Phys. Chem. Ref. Data 41 (2012) N4.
[10] J. Ruckowski, M. Elantkowska, J. Dembczynski, J. Quant. Spectrosc. Radiat. Transfer 149 (2014) 168.
[11] J. Ruckowski, S. Bouazza, M. Elantkowska, J. Dembczynski, J. Quant. Spectrosc. Radiat. Transfer 155 (2015) 1.
[12] S. Bouazza, J. Spectrosc. Radiat. Transfer 187 (2017) 280.
[13] H. Nilsson, G. Lyung, H. Lundberg, K.E. Nielsen, Astron. Astrophys. 445 (2006) 1165.
[14] J. Gurell, H. Nilsson, L. Engström, H. Lundberg, R. Blackwell-Whitehead, K.E. Nielsen, S. Mannervik, Astron. Astrophys. 511 (2010) A68.
[15] L. Engström, H. Lundberg, H. Nilsson, H. Hartman, E. Bäckström, Astron. Astrophys. 570 (2014) A34.
[16] S.D. Bergeson, J.E. Lawler, Astrophs. J. 408 (1993) (1993) 382.
[17] J. Dembczynski E. Stachowska, G. Szawiola, J. Ruckowski, Eur. Phys. J. D 4 (1998) 39.
[18] S. Bouazza, Can. J. Phys. 94 (2016) (2016) 1310.
[19] J. Dembczynski, S. Bouazza, G. Szawiola, J. Ruckowski, J. Physique 7 (1997) 1175.
[20] S. Bouazza, P. Quinet, P. Palmeri, J. Quant. Spectrosc. Radiat. Transfer 163 (2015) 39.
[21] P. Quinet, S. Bouazza, P. Palmeri, J. Quant. Spectrosc. Radiat. Transfer 164 (2015) 193.
[22] J. Dembczynski, M. Elantkowska, B. Furmann, J. Ruckowski, J. Phys. B. 43 (2010) 6.

[23] J. Dembczynski, M. Elantkowska, J. Ruckowski, D. Stefanska, At. Data Nucl. Data Tables 93 (2007) 1.

[24] J. Dembczynski, G. Szawiola, M. Elantkowska, E. Stachowska, J. Ruckowski, Phys. Scr. 54 (1996) 5.

[25] E. Stachowska, J. Dembczynski, L. Windholz, J. Ruckowski, M. Elantkowska, At. Data Nucl. Data Tables 113 (2017) 350.

[26] M. Elantkowska, J. Ruckowski, J. Dembczynski, Eur. Phys. J. Plus 130 (2015) 1.

[27] C.J. Sansonetti, G. Nave, Astrophys. J. Suppl. Ser. 213 (2014) 28.

[28] R.D. Cowan, The Theory of Atomic Structure Spectra, University of California Press, Berkeley, CA, 1981.

Explanation of Tables

Table 1.   **Comparison of the experimental and calculated energy values, percentages of first and second components and g_J-factors for Cr II even-parity configurations**

J-value:	Total angular momentum of considered level.
E_{obs}:	Observed energy level value in cm^{-1}.
E_{calc}:	Calculated eigenvalue in cm^{-1}.
Largest eigenvalue component:	Percentage contribution of the main eigenvector component. In $^{2S'+1}L'$; ^{2S+1}L, $^{2S'+1}L'$ stands for the parent term.
Next largest component:	Percentage contribution of the second eigenvector component. In $^{2S'+1}L'$; ^{2S+1}L, $^{2S'+1}L'$ stands for the parent term.
Calc. g_J:	Calculated Landé g_J-factor value using eigenvector level composition.
Obs. g_J:	Measured Landé g_J-factor value by means of Zeeman structure.

Table 2.   **Values of the intra-configuration fine structure parameters for Cr II even configurations**

Configuration:	Name ofthe considered configuration in this study.
Parameter:	Name of radial parameter.
Value:	Radial parameter value in cm^{-1}. Standard deviation is given in parentheses. ^{f} Frozen to zero. ^{d} Deduced from a b initio or fs calculations.

Table 3.   **Values of even configuration interaction parameters**

Configurations:	Designations of interacting configurations.
Parameter:	Name of radial parameter whose meanings are given in [26].
Value:	Radial parameter value in cm^{-1}. Standard deviation is given in parentheses.

Table 4   **Proposals of new positions for the quartet 3d^4(^{5}D)5d ^{4}F**

J-value:	Total angular momentum of considered level.
Position given in [27]:	Experimental energy level in cm^{-1} given in Ref. [27].
Our proposed position:	Obtained energy level in cm^{-1} by means of our calculations.

Table 5   **Comparison of the experimental and calculated energy values, percentages of first and second components and g_J-factors for Cr II odd-parity configurations**

J-value:	Total angular momentum of considered level.
E_{obs}:	Observed energy level value in cm^{-1}.
E_{calc}:	Calculated eigenvalue in cm^{-1}.
Largest eigenvalue component:	Percentage contribution of the main eigenvector component. In $^{2S'+1}L'$; ^{2S+1}L, $^{2S'+1}L'$ stands for the parent term. In 3d^{3}4s4p $^{2S''+1}L''$. $^{2S'+1}L'$; ^{2S+1}L, $^{2S'+1}L'$ and $^{2S''+1}L''$ stand respectively for the parent and grandparent terms.
Next largest component:	Percentage contribution of the second eigenvector component. In $^{2S'+1}L'$; ^{2S+1}L, $^{2S'+1}L'$ stands for the parent term. In 3d^{3}4s4p $^{2S''+1}L''$. $^{2S'+1}L'$; ^{2S+1}L, $^{2S'+1}L'$ and $^{2S''+1}L''$ stand respectively for the parent and grandparent terms.
Calc. g_J:	Calculated Landé g_J-factor value using eigenvector level composition.
Obs. g_J:	Measured Landé g_J-factor value by means of Zeeman structure.

Table 6   **Values of the intra-configuration fine structure parameters for Cr II odd configurations**

Configuration:	Name of the considered configuration in this study.
Parameter:	Name of radial parameter.
Value:	Radial parameter value in cm^{-1}. Standard deviation is given in parentheses. ^{f} Frozen to zero. ^{d} Deduced from ab initio or fs calculations.

Table 7   **Values of odd configuration interaction parameters**

Configurations:	Designations of interacting configurations.
Parameter:	Name of radial parameter whose meanings are given in [25].
Value:	Radial parameter value in cm^{-1}. Standard deviation is given in parentheses. ^{d} Deduced from ab initio or fs calculations.

Table 1
Comparison of the experimental and calculated energy values, percentages of first and second components and g_J-factors for Cr II even-parity configurations.

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
0.5								
	11961.747	11908	99.84	3d^4 4s ^{5}D; ^{6}D	0.05	3d^4 4s ^{3}P; ^{4}P	3.338	3.323
	19528.230	19510	95.21	3d^4 4s^{5}D; ^{4}D	4.34	3d^5^{4}D	−0.001	0.000
	21823.725	21873	97.05	3d^5^{4}P	1.00	3d^4 4s ^{3}P; ^{4}P	2.664	2.693
	25035.346	25062	94.12	3d^5^{4}D	4.41	3d^4 4s^{5}D; ^{4}D	0.003	0.045
	29951.818	29959	57.86	3d^4 4s ^{3}P; ^{4}P	40.32	3d^4 4s ^{3}P; ^{4}P	2.666	2.685
	34659.242	34674	58.61	3d^4 4s ^{3}P; ^{2}P	40.45	3d^4 4s ^{3}P; ^{2}P	0.671	0.67
	38396.188	38409	99.21	3d^4 4s ^{3}D; ^{4}D	0.46	3d^5^{4}D	0.000	
	40415.090	40364	53.58	3d^4 4s ^{1}S; ^{2}S	31.31	3d^5^{2}S	1.999	
	44307.078	44287	67.38	3d^5^{2}S	24.22	3d^4 4s ^{1}S; ^{2}S	2.002	
	55626.102	55655	58.96	3d^4 4s ^{3}P; ^{4}P	40.54	3d^4 4s ^{3}P; ^{4}P	2.669	
	59526.684	59491	47.13	3d^4 4s ^{3}P; ^{2}P	34.02	3d^4 4s ^{3}P; ^{2}P	0.667	
		63372	64.01	3d^5^{2}P	15.56	3d^3 4s^2^{2}P	0.671	
	65882.438	65895	98.88	3d^3 4s^2^{4}P	0.43	3d^5^{4}P	2.659	
		70925	83.11	3d^3 4s^2^{2}P	15.5	3d^5^{2}P	0.673	
	82692.008	82677	99.63	3d^4 5s^{5}D; ^{6}D	0.09	3d^4 4d^{5}D; ^{6}D	3.337	
	84209.781	84218	99.72	3d^4 5s^{5}D; ^{4}D	0.09	3d^4 4s^{5}D; ^{4}D	0.000	
	87453.484	87368	95.41	3d^4 4d^{5}D; ^{6}D	3.88	3d^4 4d^{5}D; ^{6}F	3.180	
	87594.562	87615	95.5	3d^4 4d^{5}D; ^{6}F	3.89	3d^4 4d^{5}D; ^{6}D	−0.512	
	89254.469	89246	89.28	3d^4 4d^{5}D; ^{4}P	7.14	3d^4 4d^{5}D; ^{4}D	2.474	
	89651.617	89559	89.27	3d^4 4d^{5}D; ^{4}D	7.14	3d^4 4d^{5}D; ^{4}P	0.195	
		94771	77.64	3d^4 4s ^{1}S; ^{2}S	21.51	3d^4 4s ^{1}S; ^{2}S	2.002	
	99677.850	99706	59.62	3d^4 5s ^{3}P; ^{4}P	37.31	3d^4 5s ^{3}P; ^{4}P	2.617	
	100782.820	100809	59.92	3d^4 5s ^{3}P; ^{2}P	37.06	3d^4 5s ^{3}P; ^{2}P	0.719	
	105098.859	105135	99.7	3d^4 6s^{5}D; ^{6}D	0.13	3d^4 6s^{5}D; ^{4}D	3.334	
		105797	56.83	3d^4 4d ^{3}F; ^{4}D	11.94	3d^4 6s^{5}D; ^{4}D	0.018	
	105923.445	105862	87.2	3d^4 6s^{5}D; ^{4}D	6.41	3d^4 4d ^{3}F; ^{4}D	0.006	
	.							
	.							
	115234.461	115235	98.73	3d^4 7s ^{5}D; ^{6}D	1.04	3d^4 7s ^{5}D; ^{4}D	3.303	
		115527	98.77	3d^4 7s ^{5}D; ^{4}D	1.04	3d^4 7s^{5}D; ^{6}D	0.033	
	116361.016	116348	77.29	3d^4 6d^{5}D; ^{6}F	21.6	3d^4 6d^{5}D; ^{6}D	0.208	
	.							
	.							
	120702.898	120699	96.61	3d^4 8s ^{5}D; ^{6}D	3.15	3d^4 8s ^{5}D; ^{4}D	3.233	
1.5								
	12032.545	11980	99.86	3d^4 4s^{5}D; ^{6}D	0.03	3d^4 4s ^{3}P; ^{4}P	1.869	1.867
	19631.205	19614	94.97	3d^4 4s^{5}D; ^{4}D	4.54	3d^5^{4}D	1.201	1.192
	21824.141	21865	96.65	3d^5^{4}P	0.92	3d^4 4s ^{3}P; ^{4}P	1.731	1.717
	25042.760	25074	93.5	3d^5^{4}D	4.52	3d^4 4s^{5}D; ^{4}D	1.204	1.207
	30307.365	30311	58.16	3d^4 4s ^{3}P; ^{4}P	40.22	3d^4 4s ^{3}P; ^{4}P	1.734	1.756
	31082.885	31134	65.91	3d^4 4s ^{3}F; ^{4}F	19.35	3d^4 4s ^{3}F; ^{4}F	0.414	0.416
	31531.172	31496	67.93	3d^5^{2}D	23.09	3d^5^{2}D	0.776	
	32844.703	33029	84.75	3d^5^{4}F	6.86	3d^4 4s ^{3}F; ^{4}F	0.408	
	35355.898	35374	59.03	3d^4 4s ^{3}P; ^{2}P	40.25	3d^4 4s ^{3}P; ^{2}P	1.334	1.331
	38362.383	38383	99.09	3d^4 4s ^{3}D; ^{4}D	0.47	3d^5^{4}D	1.201	
	42986.566	43026	92.93	3d^4 4s ^{3}D; ^{2}D	4.32	3d^5^{2}D	0.800	
	45669.398	45634	64.69	3d^4 4s ^{1}D; ^{2}D	17.43	3d^4 4s ^{1}D; ^{2}D	0.800	
	47372.430	47317	75.78	3d^5^{2}D	12.38	3d^4 4s ^{1}D; ^{2}D	0.800	
	53051.270	53055	97.64	3d^3 4s^2^{4}F	2.09	3d^5^{4}F	0.399	
	54868.508	54894	76.42	3d^4 4s ^{3}F; ^{4}F	23.02	3d^4 4s ^{3}F; ^{4}F	0.399	
	55398.672	55424	59	3d^4 4s ^{3}P; ^{4}P	40.4	3d^4 4s ^{3}P; ^{4}P	1.734	
	59130.340	59117	49.13	3d^4 4s ^{3}P; ^{2}P	34.96	3d^4 4s ^{3}P; ^{2}P	1.335	
		63311	66.68	3d^5^{2}D	15.1	3d^3 4s^2^{2}P	1.334	
	66010.273	66001	97.86	3d^3 4s^2^{4}P	1.03	3d^5^{2}P	1.728	
	.							
	.							
	82763.664	82749	99.57	3d^4 5s^{5}D; ^{6}D	0.12	3d^4 5s^{5}D; ^{4}D	1.868	
	84320.141	84329	99.67	3d^4 5s^{5}D; ^{4}D	0.13	3d^4 5s^{5}D; ^{6}D	1.201	
	86165.266	86097	95.35	3d^4 4d^{5}D; ^{4}S	3.49	3d^4 4d^{5}D; ^{6}P	2.015	
	86594.375	86527	99.02	3d^4 4d^{5}D; ^{6}G	0.44	3d^4 5d^{5}D; ^{6}G	0.002	
	86667.719	86683	94.39	3d^4 4d^{5}D; ^{6}P	3.51	3d^4 4d^{5}D; ^{4}S	2.381	
	87470.539	87397	86.55	3d^4 4d^{5}D; ^{6}D	11.37	3d^4 4d^{5}D; ^{6}F	1.783	
	87666.203	87681	87.76	3d^4 4d^{5}D; ^{6}F	11.34	3d^4 4d^{5}D; ^{6}D	1.157	
	89277.922	89264	79.68	3d^4 4d^{5}D; ^{4}P	16.3	3d^4 4d^{5}D; ^{4}D	1.645	
	89724.172	89648	79.19	3d^4 4d^{5}D; ^{4}D	16.3	3d^4 4d^{5}D; ^{4}P	1.283	
	90512.516	90566	94.39	3d^4 4d^{5}D; ^{4}F	1.23	3d^4 4d ^{3}H; ^{4}F	0.407	
		99957	75.4	3d^3 4s^2^{2}D	22.79	3d^4 4s^{1}S ; ^{2}D	0.800	
	100040.172	100052	59.72	3d^4 5s ^{3}P; ^{4}P	37	3d^4 5s ^{3}P; ^{4}P	1.722	
	101245.000	101207	79.67	3d^4 5s ^{3}F; ^{4}F	20.08	3d^4 5s ^{3}F; ^{4}F	0.399	

Table 1 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	101492.820	101511	60.1	3d^4 5s ^{3}P; ^{2}P	36.5	3d^4 5s ^{3}P; ^{2}P	1.346	
		104266	78.85	3d^4 4d ^{3}H; ^{4}F	6.79	3d^4 4d ^{3}G; ^{4}F	0.406	
	105168.766	105228	19.21	3d^4 4d ^{3}P; ^{4}F	18.29	3d^4 4d ^{3}P; ^{4}D	0.921	
		105508	28.96	3d^4 4d ^{3}P; ^{4}F	18.17	3d^4 4d ^{3}P; ^{4}F	0.786	
		105592	19.93	3d^4 4d ^{3}F; ^{2}P	18.23	3d^4 4d ^{3}F; ^{4}D	1.232	
	105980.445	106013	26.94	3d^4 4d ^{3}F; ^{4}P	17.46	3d^4 4d ^{3}P; ^{4}P	1.530	
		106216	26.42	3d^4 4d ^{3}F; ^{4}F	14.16	3d^4 4d ^{3}F; ^{4}P	1.073	
		106306	39.88	3d^4 4d ^{3}F; ^{4}F	9.79	3d^4 5d^{5}D; ^{4}P	0.829	
		106596	33.33	3d^4 4d ^{3}P; ^{2}D	15.2	3d^4 4d ^{3}P; ^{2}D	0.879	
		106626	99.01	3d^4 6s ^{5}D; ^{6}D	0.4	3d^4 6s^{5}D; ^{4}D	1.863	
	106627.164	106664	28.02	3d^4 5d^{5}D; ^{4}P	22.57	3d^4 4d ^{3}P; ^{4}P	1.578	
	106877.172	106879	95.31	3d^4 5d^{5}D; ^{6}G	2.15	3d^4 5d^{5}D; ^{6}F	0.032	
		106952	64.67	3d^4 5d ^{5}D; ^{6}P	20.48	3d^4 5d^{5}D; ^{4}S	2.219	
	106924.797	107096	51.23	3d^4 5d^{5}D; ^{4}S	14.86	3d^4 5d^{5}D; ^{6}P	1.853	
		107138	31.97	3d^4 4d ^{3}G; ^{4}D	21.71	3d^4 5d^{5}D; ^{4}D	1.257	
		107162	44.51	3d^4 4d ^{3}G; ^{4}F	28.8	3d^4 5d^{5}D; ^{4}F	0.640	
	107259.820	107231	52.53	3d^4 5d^{5}D; ^{6}F	20.9	3d^4 5d^{5}D; ^{6}D	1.315	
		107392	58.27	3d^4 6s^{5}D; ^{4}D	11.19	3d^4 4d ^{3}P; ^{2}P	1.232	
	107414.688	107407	50.59	3d^4 5d^{5}D; ^{6}D	25.75	3d^4 5d^{5}D; ^{6}F	1.570	
		107435	27.61	3d^4 6s^{5}D; ^{4}D	12.61	3d^4 4d ^{3}F; ^{2}P	1.301	
	107516.711	107967	96.26	3d^4 5s ^{3}D; ^{4}D	1.75	3d^4 4d ^{3}G; ^{4}D	1.199	
		108182	83.06	3d^4 5s ^{3}G; ^{2}D	9.18	3d^4 4d ^{3}D; ^{2}D	0.826	
		108717	46.9	3d^4 4d ^{3}F; ^{2}D	11.96	3d^4 5s ^{3}D; ^{2}D	0.798	
	. .							
	115301.977	115301	97.15	3d^4 7s ^{5}D; ^{6}D	2.64	3d^4 7s ^{5}D; ^{4}D	1.851	
	115640.297	115641	97.21	3d^4 7s^{5}D; ^{4}D	2.64	3d^4 7s^{5}D; ^{6}D	1.218	
	116171.633	116191	90.96	3d^4 6d^{5}D; ^{6}G	6.41	3d^4 6d^{5}D; ^{6}F	0.095	
	116253.273	116281	46.32	3d^4 6d^{5}D; ^{6}P	27.68	3d^4 6d^{5}D; ^{6}D	2.005	
	116355.430	116383	52.81	3d^4 6d^{5}D; ^{4}S	21.83	3d^4 6d^{5}D; ^{6}P	1.892	
	116429.156	116444	49.19	3d^4 6d^{5}D; ^{6}F	28.83	3d^4 6d^{5}D; ^{4}S	1.487	
	116581.773	116567	58.46	3d^4 6d^{5}D; ^{6}D	22.01	3d^4 6d^{5}D; ^{6}P	1.850	
		117106	84.21	3d^4 6d^{5}D; ^{4}F	2.88	3d^4 6d^{5}D; ^{4}D	0.447	
		117191	56.2	3d^4 4d ^{1}S; ^{2}D	14.02	3d^4 4d ^{1}S; ^{2}D	0.825	
	117381.578	117348	56.31	3d^4 6d^{5}D; ^{4}P	17.7	3d^4 6d^{5}D; ^{4}D	1.539	
		117637	55.04	3d^4 6d^{5}D; ^{4}D	22.16	3d^4 6d^{5}D; ^{4}P	1.332	
2.5	0.000	−307	99.87	3d^5 ^{6}S	0.06	3d^4 5d^{5}D; ^{6}S	2.002	
	12147.772	12100	99.88	3d^4 4s^{5}D; ^{6}D	0.03	3d^4 6s^{5}D; ^{6}D	1.659	1.669
	19797.859	19783	94.63	3d^4 4s^{5}D; ^{4}D	4.85	3d^5^{4}D	1.373	1.37
	20512.062	20529	98.83	3d^5^{4}G	0.4	3d^4 4s ^{3}G; ^{4}G	0.571	0.599
	21822.506	21857	96.32	3d^5^{4}P	0.83	3d^4 4s ^{3}P; ^{4}P	1.598	1.59
	25046.715	25081	92.97	3d^5^{4}D	4.78	3d^4 4s^{5}D; ^{4}D	1.374	1.381
	30864.434	30878	58.38	3d^4 4s ^{3}P; ^{4}P	39.96	3d^4 4s ^{3}P; ^{4}P	1.599	1.572
	31117.326	31162	60.79	3d^4 4s ^{3}F; ^{4}F	17.62	3d^4 4s ^{3}F; ^{4}F	1.039	1.032
	31350.875	31306	51.78	3d^5^{2}D	17.62	3d^5^{2}D	1.125	
	32603.355	32547	78.45	3d^5^{2}F	12.63	3d^5^{2}D	0.919	
	32854.941	33015	83.19	3d^5^{4}F	6.57	3d^4 4s ^{3}F; ^{4}F	1.023	
	33417.980	33417	96.55	3d^4 4s ^{3}G; ^{4}G	1.15	3d^4 4s ^{3}F; ^{4}F	0.583	0.588
	35569.180	35619	67.69	3d^4 4s ^{3}F; ^{2}F	19.27	3d^4 4s ^{3}F; ^{2}F	0.856	0.876
	38314.836	38344	99.11	3d^4 4s ^{3}D; ^{4}D	0.47	3d^5^{4}D	1.372	
	39742.035	39725	86.3	3d^5^{2}F	8.06	3d^4 4s ^{3}F; ^{2}F	0.857	
	42897.945	42928	91.5	3d^4 4s ^{3}D; ^{2}D	4.89	3d^5^{2}D	1.200	
	45730.598	45712	65.75	3d^4 4s ^{1}D; ^{2}D	17.78	3d^4 4s ^{1}D; ^{2}D	1.201	
	47354.371	47306	79.1	3d^5^{2}D	10.63	3d^4 4s ^{1}D; ^{2}D	1.200	
	50687.621	50622	98.56	3d^4 4s ^{1}F; ^{2}F	0.6	3d^5^{2}F	0.858	
	53271.008	53273	97.7	3d^3 4s^2^{4}F	2.05	3d^5^{4}F	1.029	
	54883.496	54897	76.44	3d^4 4s ^{3}F; ^{4}F	22.65	3d^4 4s ^{3}F; ^{4}F	1.028	
	55023.027	55055	59.3	3d^4 4s ^{3}P; ^{4}P	40.2	3d^4 4s ^{3}P; ^{4}P	1.601	
	59577.660	59634	76.34	3d^4 4s ^{3}F; ^{2}F	22.81	3d^4 4s ^{3}F; ^{2}F	0.857	
	66256.578	66225	98	3d^3 4s^2^{4}P	0.61	3d^5^{2}D	1.595	
		67161	55.12	3d^5 ^{2}D	21.14	3d^5^{2}D	1.206	
		72416	66.62	3d^3 4s^2^{2}D	14.16	3d^3 4s^2^{2}D	1.201	
		77494	76.71	3d^4 4s ^{1}D; ^{2}D	22.31	3d^4 4s ^{1}D; ^{2}D	1.200	
	82881.094	82868	99.53	3d^4 5s^{5}D; ^{6}D	0.19	3d^4 5s^{5}D; ^{4}D	1.658	
		82905	99.53	3d^3 4s^2^{2}F	0.33	3d^5^{2}F	0.857	
	84495.609	84509	99.63	3d^4 5s^{5}D; ^{4}D	0.19	3d^4 5s^{5}D; ^{6}D	1.373	
	86654.172	86551	98.6	3d^4 4d^{5}D; ^{6}G	0.72	3d^4 4d^{5}D; ^{6}F	0.860	
	86691.516	86744	96.36	3d^4 4d^{5}D; ^{6}P	2.83	3d^4 4d^{5}D; ^{6}D	1.881	
	87514.797	87451	79.59	3d^4 4d^{5}D; ^{6}D	17.09	3d^4 4d^{5}D; ^{6}F	1.603	

Table 1 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	87759.062	87773	81.67	3d^4 4d^{5}D; ^{6}F	17.06	3d^4 4d^{5}D; ^{6}D	1.373	
	89055.945	89169	96.39	3d^4 4d^{5}D; ^{4}G	1.22	3d^4 4d ^{3}H; ^{4}G	0.573	
	89336.812	89326	79.19	3d^4 4d^{5}D; ^{4}P	17.19	3d^4 4d^{5}D; ^{4}D	1.559	
	89812.398	89746	77.45	3d^4 4d^{5}D; ^{4}D	17.34	3d^4 4d^{5}D; ^{4}P	1.407	
	90608.961	90670	93.23	3d^4 4d^{5}D; ^{4}F	1.93	3d^4 4d^{5}D; ^{4}D	1.034	
	91955.336	91949	91.84	3d^4 4d^{5}D; ^{6}S	6.41	3d^4 5d^{5}D; ^{6}S	2.002	
		99783	76.65	3d^3 4s^2 ^{2}D	21.47	3d^3 4s^2 ^{2}D	1.200	
	100650.461	100659	61.93	3d^4 5s ^{3}P; ^{4}P	37.79	3d^4 6s ^{3}P; ^{4}P	1.601	
	101276.547	101235	79.23	3d^4 5s ^{3}F; ^{4}F	19.72	3d^4 6s ^{3}F; ^{4}F	1.025	
	102148.703	102139	78.25	3d^4 5s ^{3}F; ^{2}F	19.47	3d^4 6s ^{3}F; ^{2}F	0.852	
		103444	96.84	3d^4 5s ^{3}G; ^{4}G	1.58	3d^4 6s ^{3}F; ^{2}F	0.580	
		104299	78.29	3d^4 4d ^{3}H; ^{4}F	7.64	3d^4 4d ^{3}G; ^{4}F	1.030	
		104893	74.29	3d^4 4d ^{3}H; ^{4}G	12.45	3d^4 5d^{5}D; ^{4}G	0.588	
		105108	65.4	3d^4 4d ^{3}H; ^{2}F	10.44	3d^4 4d ^{3}P; ^{2}F	0.901	
	105285.312	105358	21.34	3d^4 4d ^{3}P; ^{4}D	17.84	3d^4 4d ^{3}F; ^{4}D	1.231	
		105690	30.06	3d^4 4d ^{3}P; ^{4}F	18.89	3d^4 4d ^{3}P; ^{4}F	1.153	
	105923.438	105897	24.22	3d^4 4d ^{3}P; ^{4}P	20.19	3d^4 4d ^{3}F; ^{4}P	1.508	
	106095.602	106065	63.97	3d^4 4d ^{3}F; ^{4}G	14.46	3d^4 5d^{5}D; ^{4}G	0.576	
		106244	38.39	3d^4 4d ^{3}F; ^{4}F	9.41	3d^4 4d ^{3}F; ^{4}P	1.214	
		106388	22.07	3d^4 4d ^{3}F; ^{4}F	19.43	3d^4 5d^{5}D; ^{4}P	1.316	
	106722.555	106649	15.01	3d^4 5d^{5}D; ^{4}P	13.36	3d^4 4d ^{3}P; ^{4}D	1.351	
		106726	98.22	3d^4 5d ^{5}D; ^{6}D	0.55	3d^4 6s^{5}D; ^{4}D	1.652	
		106741	26.58	3d^4 4d ^{3}P; ^{2}D	12.75	3d^4 4d ^{3}F; ^{2}D	1.304	
	106929.375	106929	86.28	3d^4 5d^{5}D; ^{6}G	5.45	3d^4 5d^{5}D; ^{6}F	0.905	
		106970	51.58	3d^4 4d ^{3}F; ^{2}F	10.97	3d^4 4d ^{3}F; ^{2}F	0.851	
	107025.250	107002	73.12	3d^4 5d^{5}D; ^{6}P	18.77	3d^4 5d^{5}D; ^{6}D	1.789	
		107233	43.92	3d^4 4d ^{3}G; ^{4}D	31.85	3d^4 5d^{5}D; ^{4}D	1.370	
		107254	38.15	3d^4 5d ^{5}D; ^{6}F	20.05	3d^4 4d ^{3}G; ^{4}F	1.268	
	107309.328	107291	47.23	3d^4 4d ^{3}G; ^{4}G	27.69	3d^4 5d^{5}D; ^{4}G	0.663	
		107321	30.79	3d^4 4d ^{3}G; ^{4}F	20.09	3d^4 5d^{5}D; ^{4}F	1.199	
	107519.422	107521	56.94	3d^4 5d^{5}D; ^{6}D	31.07	3d^4 5d^{5}D; ^{6}F	1.554	
	107597.609	107556	93.54	3d^4 6s^{5}D; ^{4}D	2.38	3d^4 4d ^{3}G; ^{4}D	1.376	
		107888	35.14	3d^4 4d ^{3}G; ^{2}F	21.56	3d^4 4d ^{3}P; ^{2}F	0.885	
	107726.773	107931	92.97	3d^4 5s ^{3}D; ^{4}D	2.25	3d^4 4d ^{3}G; ^{4}D	1.359	
		108219	71.69	3d^4 4d ^{3}G; ^{2}D	6.9	3d^4 4d ^{3}F; ^{2}D	1.193	
		108780	75.41	3d^4 5s ^{3}D; ^{2}D	9.19	3d^4 4d ^{3}F; ^{2}D	1.200	
		108875	33.65	3d^4 4d ^{3}F; ^{2}D	23.46	3d^4 5s ^{3}D; ^{2}D	1.191	
		109135	44.94	3d^4 4d ^{3}G; ^{2}F	19.13	3d^4 4d ^{3}P; ^{2}F	0.871	
		110092	20.48	3d^4 4d ^{3}D; ^{4}D	19.71	3d^4 4d ^{3}G; ^{4}D	1.352	
		110324	31.92	3d^4 5d ^{5}D; ^{4}F	18.21	3d^4 4d ^{3}D; ^{4}F	1.136	
		110431	21.12	3d^4 5d^{5}D; ^{4}P	17.86	3d^4 4d ^{3}D; ^{4}P	1.505	
		110873	26.93	3d^4 5d^{5}D; ^{4}G	26.3	3d^4 4d ^{3}G; ^{4}G	0.578	
	109394.430	111469	80.84	3d^4 5d^{5}D; ^{6}S	15.35	3d^4 6d^{5}D; ^{6}S	2.002	
		112672	71.79	3d^4 4d ^{3}D; ^{4}F	9	3d^4 4d ^{3}G; ^{4}F	1.018	
		112888	48.81	3d^4 4d ^{3}D; ^{4}G	24.55	3d^4 4d ^{3}D; ^{2}F	0.695	
		113025	37.65	3d^4 4d ^{3}D; ^{2}F	30.86	3d^4 4d ^{3}D; ^{4}G	0.749	
		113505	61.82	3d^4 4d ^{3}D; ^{4}P	10.14	3d^4 6d^{5}D; ^{4}P	1.577	
		113851	36.13	3d^4 5s ^{1}D; ^{2}D	21.94	3d^4 4d ^{1}G; ^{2}D	1.214	
		113911	29.21	3d^4 5s ^{1}D; ^{2}D	28.51	3d^4 4d ^{3}D; ^{4}D	1.299	
		113972	20.76	3d^4 4d ^{1}G; ^{2}D	18.56	3d^4 4d ^{3}D; ^{4}D	1.281	
		114340	58.72	3d^4 4d ^{3}D; ^{2}D	15.23	3d^4 4d ^{1}S; ^{2}D	1.200	
	115417.797	115416	96.77	3d^4 7s^{5}D; ^{6}D	3.05	3d^4 7s^{5}D; ^{4}D	1.650	
	115818.391	115818	96.82	3d^4 7s^{5}D; ^{4}D	3.04	3d^4 7s^{5}D; ^{6}D	1.381	
	116213.320	116227	75.63	3d^4 6d^{5}D; ^{6}G	15.12	3d^4 6d^{5}D; ^{6}F	0.996	
		116304	29.33	3d^4 4d ^{1}G; ^{2}F	24.34	3d^4 4d ^{3}D; ^{2}F	0.940	
	116294.969	116308	38.81	3d^4 6d^{5}D; ^{6}P	30.27	3d^4 6d^{5}D; ^{6}D	1.534	
	116477.406	116466	58.21	3d^4 6d^{5}D; ^{6}F	31.59	3d^4 6d^{5}D; ^{6}P	1.470	
	116687.078	116670	58.12	3d^4 6d^{5}D; ^{6}D	21.07	3d^4 6d^{5}D; ^{6}P	1.636	
	116877.070	116951	79.87	3d^4 6d^{5}D; ^{4}G	7.13	3d^4 6d^{5}D; ^{4}F	0.611	
	117072.742	117156	55.39	3d^4 4d ^{1}S; ^{2}D	13.83	3d^4 4d ^{1}S; ^{2}D	1.213	
	117228.406	117193	71.98	3d^4 6d^{5}D; ^{4}F	6.87	3d^4 6d^{5}D; ^{4}G	1.035	
	117481.172	117400	58.37	3d^4 6d^{5}D; ^{4}P	13.7	3d^4 6d^{5}D; ^{4}D	1.499	
		117729	56.56	3d^4 6d^{5}D; ^{4}D	20.18	3d^4 6d^{5}D; ^{4}P	1.415	
		118772	99.38	3d^4 6s ^{1}F; ^{2}F	0.14	3d^4 5s ^{3}F; ^{4}F	0.857	
		119678	66.44	3d^4 4d ^{1}D; ^{2}F	17.53	3d^4 4d ^{1}D; ^{2}F	0.865	
		119789	82.92	3d^4 6d ^{5}D; ^{6}S	12.34	3d^4 5d^{5}D; ^{6}S	2.002	
	117672.453	120129	64.41	3d^4 4d ^{1}D; ^{2}D	15.96	3d^4 4d ^{1}D; ^{2}D	1.193	
	120870.633	120874	93.6	3d^4 8s^{5}D; ^{6}D	6.2	3d^4 8s^{5}D; ^{4}D	1.641	
		121156	93.73	3d^4 8s^{5}D; ^{4}D	6.2	3d^4 8s^{5}D; ^{6}D	1.390	
3.5								

Table 1 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	12303.820	12263	99.89	3d^4 4s ^{5}D; ^{6}D	0.03	3d^4 5s ^{5}D; ^{6}D	1.589	1.578
	20024.012	20015	94.44	3d^4 4s ^{5}D; ^{4}D	5.17	3d^{54}D	1.429	1.427
	20517.793	20539	98.91	3d^{54}G	0.39	3d^4 4s ^{3}G; ^{4}G	0.984	0.994
	25033.668	25064	93.27	3d^{54}D	5.27	3d^4 4s^{5}D; ^{4}D	1.429	1.432
	30156.732	30166	99.33	3d^4 4s ^{3}H; ^{4}H	0.33	3d^4 4s ^{3}G; ^{4}G	0.668	0.667
	31168.576	31221	68.49	3d^4 4s ^{3}F; ^{4}F	19.52	3d^4 4s ^{3}F; ^{4}F	1.235	1.246
	32355.656	32325	97.72	3d^{52}F	0.44	3d^4 4s ^{3}F; ^{2}F	1.143	
	32836.656	33002	84.5	3d^{54}F	7.03	3d^4 4s ^{3}F; ^{4}F	1.233	
	33521.090	33530	95.73	3d^4 4s ^{3}G; ^{4}G	1.81	3d^4 4s ^{3}F; ^{4}F	0.992	1.024
	35607.512	35657	66.93	3d^4 4s ^{3}F; ^{2}F	18.26	3d^4 4s ^{3}F; ^{2}F	1.138	1.144
	36101.527	36130	74.33	3d^{52}G	17.3	3d^4 4s ^{3}G; ^{2}G	0.890	
	38269.570	38302	99.28	3d^4 4s ^{3}D; ^{4}D	0.48	3d^{54}D	1.429	
	38508.934	38494	76.87	3d^4 4s ^{3}G; ^{2}G	10.88	3d^{52}G	0.894	0.91
	39683.719	39638	32.57	3d^4 4s ^{1}G; ^{2}G	32.08	3d^{52}F	0.979	
	39877.035	39823	52.62	3d^{52}F	20.25	3d^4 4s ^{1}G; ^{2}G	1.052	
	50667.234	50611	98.44	3d^4 4s ^{1}F; ^{2}F	0.57	3d^{52}F	1.144	
	52297.766	52192	91.94	3d^{52}G	4.64	3d^3 4s^{22}G	0.889	
	53566.262	53572	97.59	3d^3 4s^{24}F	2	3d^{54}F	1.238	
	54887.986	54884	76.69	3d^4 4s ^{3}F; ^{4}F	22.21	3d^4 4s ^{3}F; ^{4}F	1.238	
	59570.199	59595	76.87	3d^4 4s ^{3}F; ^{2}F	21.95	3d^4 4s ^{3}F; ^{2}F	1.142	
	62701.734	62582	64.29	3d^4 4s ^{1}G; ^{2}G	34.24	3d^4 4s ^{1}G; ^{2}G	0.889	
		65898	94.52	3d^3 4s^{22}G	4.65	3d^{52}G	0.889	
		82767	99.57	3d^3 4s^{22}F	0.33	3d^{52}F	1.143	
	83041.320	83033	99.57	3d^4 5s^{5}D; ^{6}D	0.16	3d^4 5s^{5}D; ^{4}D	1.588	
	84726.680	84749	99.63	3d^4 5s^{5}D; ^{4}D	0.16	3d^4 5s^{5}D; ^{6}D	1.430	
	86738.273	86646	98.21	3d^4 4d^{5}D; ^{6}G	1.09	3d^4 4d^{5}D; ^{6}F	1.146	
	86782.047	86832	96.26	3d^4 4d^{5}D; ^{6}P	2.98	3d^4 4d^{5}D; ^{6}D	1.712	
	87587.867	87530	77.43	3d^4 4d^{5}D; ^{6}D	19.02	3d^4 4d^{5}D; ^{6}F	1.554	
	87858.469	87879	79.4	3d^4 4d^{5}D; ^{6}F	19.12	3d^4 4d^{5}D; ^{6}D	1.433	
	89173.992	89297	96.22	3d^4 4d^{5}D; ^{4}G	1.23	3d^4 4d ^{3}H; ^{4}G	0.986	
	89885.008	89808	94.8	3d^4 4d^{5}D; ^{4}D	1.81	3d^4 4d^{5}D; ^{4}F	1.426	
	90725.812	90799	93.16	3d^4 4d^{5}D; ^{4}F	1.87	3d^4 4d^{5}D; ^{4}D	1.241	
	100068.859	100073	99.18	3d^4 5s ^{3}H; ^{4}H	0.32	3d^4 5s ^{3}G; ^{4}G	0.668	
	101321.812	101276	78.98	3d^4 5s ^{3}F; ^{4}F	19.25	3d^4 5s ^{3}F; ^{4}F	1.235	
	102243.156	102225	78.7	3d^4 5s ^{3}F; ^{2}F	18.72	3d^4 5s ^{3}F; ^{2}F	1.138	
		103523	96.52	3d^4 5s ^{3}G; ^{4}G	1.22	3d^4 5s ^{3}F; ^{4}F	0.987	
	103949.273	103709	94.86	3d^4 4d ^{3}H; ^{4}H	2.88	3d^4 4d ^{3}H; ^{2}G	0.676	
		104165	71.44	3d^4 4d ^{3}H; ^{2}G	10.29	3d^4 4d ^{3}G; ^{2}G	0.906	
		104363	72.38	3d^4 4d ^{3}H; ^{4}F	7.84	3d^4 4d ^{3}G; ^{4}F	1.212	
	104543.109	104453	94.46	3d^4 5s ^{3}G; ^{2}G	1.89	3d^4 4d ^{3}H; ^{2}G	0.895	
	105198.992	104984	76.23	3d^4 4d ^{3}H; ^{4}G	12.24	3d^4 5d^{5}D; ^{4}G	0.989	
	105446.994	105436	99.42	3d^4 6s^{5}D; ^{6}D	0.45	3d^4 6s^{5}D; ^{4}D	1.588	
		105822	82.86	3d^4 4d ^{3}H; ^{2}F	7.56	3d^4 4d ^{3}P; ^{2}F	1.147	
		105857	66.47	3d^4 4d ^{3}F; ^{4}D	11.9	3d^4 4d ^{3}F; ^{4}D	1.421	
		106043	77.73	3d^4 4d ^{3}F; ^{4}H	15.05	3d^4 4d ^{3}F; ^{4}H	0.674	
		106097	38.56	3d^4 4d ^{3}F; ^{4}F	31.01	3d^4 4d ^{3}F; ^{4}G	1.115	
	106030.914	106133	60.62	3d^4 4d ^{3}F; ^{4}G	14.89	3d^4 5d^{5}D; ^{4}G	0.977	
	106275.180	106286	21.23	3d^4 4d ^{3}P; ^{4}D	18.61	3d^4 4d ^{3}P; ^{4}F	1.334	
		106575	38.38	3d^4 4d ^{3}F; ^{4}F	13.26	3d^4 4d ^{3}P; ^{4}D	1.303	
	107006.266	107009	84.49	3d^4 5d^{5}D; ^{6}G	8.21	3d^4 5d^{5}D; ^{6}F	1.186	
	107114.727	107089	68.73	3d^4 5d^{5}D; ^{6}P	18.79	3d^4 5d^{5}D; ^{6}D	1.641	
		107125	48.25	3d^4 4d ^{3}F; ^{2}F	9.95	3d^4 4d ^{3}F; ^{2}F	1.092	
		107303	45.07	3d^4 4d ^{3}G; ^{4}D	35.87	3d^4 5d^{5}D; ^{4}D	1.419	
	107386.188	107349	43.49	3d^4 5d^{5}D; ^{6}F	16.27	3d^4 5d^{5}D; ^{6}P	1.424	
		107362	46.01	3d^4 4d ^{3}F; ^{2}G	10.86	3d^4 4d ^{3}F; ^{2}G	0.934	
	107500.344	107395	51.21	3d^4 4d ^{3}G; ^{4}G	27.58	3d^4 5d^{5}D; ^{4}G	1.013	
		107455	41.46	3d^4 4d ^{3}G; ^{4}F	27.74	3d^4 5d^{5}D; ^{4}F	1.276	
	107627.367	107624	56.18	3d^4 5d^{5}D; ^{6}D	34.07	3d^4 5d^{5}D; ^{6}F	1.526	
	107716.266	107755	96.86	3d^4 6s^{5}D; ^{4}D	0.99	3d^4 5s ^{3}D; ^{4}D	1.430	
	107829.508	107825	82.64	3d^4 4d ^{3}G; ^{4}H	7.39	3d^4 4d ^{3}F; ^{2}G	0.697	
		107892	94.26	3d^4 5s ^{3}D; ^{4}D	2.92	3d^4 4d ^{3}G; ^{4}D	1.429	
		108186	48.86	3d^4 4d ^{3}G; ^{2}F	20.33	3d^4 4d ^{3}P; ^{2}F	1.141	
		108816	66.04	3d^4 5s ^{1}G; ^{2}G	33.14	3d^4 5s ^{1}G; ^{2}G	0.889	
		109400	39.21	3d^4 4d ^{3}G; ^{2}F	25.05	3d^4 4d ^{3}P; ^{2}F	1.144	
		110276	20.19	3d^4 4d ^{3}D; ^{4}D	17.12	3d^4 4d ^{3}G; ^{4}D	1.358	
	107850.555	110443	24.62	3d^4 5d^{5}D; ^{4}F	17.32	3d^4 4d ^{3}D; ^{4}F	1.300	
		110647	63.26	3d^4 4d ^{3}G; ^{2}G	7.07	3d^4 4d ^{3}H; ^{2}G	0.894	
		110919	26.82	3d^4 5d ^{5}D; ^{4}G	25.17	3d^4 4d ^{3}G; ^{4}G	0.989	
		112697	56.6	3d^4 4d ^{3}D; ^{4}F	7.84	3d^4 4d ^{3}G; ^{4}F	1.170	
		112728	36.99	3d^4 4d ^{1}I; ^{2}G	36.45	3d^4 4d ^{3}D; ^{2}G	0.949	

Table 1 (continued)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
		112924	59.71	3d^4 4d ^{3}D; ^{4}G	12.73	3d^4 4d ^{3}D; ^{2}F	1.026	
		113033	45.83	3d^4 4d ^{3}D; ^{2}F	16.96	3d^4 4d ^{1}G; ^{2}F	1.111	
		113896	55.78	3d^4 4d ^{3}D; ^{4}D	16.76	3d^4 6d^{5}D; ^{4}D	1.429	
		113997	54.99	3d^4 4d ^{1}G; ^{2}G	29.75	3d^4 4d ^{1}G; ^{2}G	0.889	
		114951	43.04	3d^4 4d ^{3}D; ^{2}G	41.96	3d^4 4d ^{1}I; ^{2}G	0.889	
	115581.641	115580	97.78	3d^4 7s^{5}D; ^{6}D	2.04	3d^4 7s^{5}D; ^{4}D	1.585	
	116047.820	116050	97.8	3d^4 7s^{5}D; ^{4}D	2.04	3d^4 7s^{5}D; ^{6}D	1.433	
		116203	32.75	3d^4 4d ^{1}G; ^{2}F	29.59	3d^4 4d ^{3}D; ^{2}F	1.143	
	116281.860	116288	68.03	3d^4 6d^{5}D; ^{6}G	20	3d^4 6d^{5}D; ^{6}F	1.245	
	116385.570	116384	39.96	3d^4 6d^{5}D; ^{6}P	33.36	3d^4 6d^{5}D; ^{6}D	1.538	
	116572.391	116550	51.7	3d^4 8s^{5}D; ^{6}F	35.86	3d^4 6d^{5}D; ^{6}P	1.492	
	116790.258	116762	56.46	3d^4 6d^{5}D; ^{6}D	21.91	3d^4 6d^{5}D; ^{6}F	1.567	
	116985.359	117046	77.99	3d^4 6d^{5}D; ^{4}G	9.46	3d^4 6d^{5}D; ^{4}F	1.013	
	117263.375	117323	73.62	3d^4 6d^{5}D; ^{4}D	6.41	3d^4 4d ^{3}D; ^{4}D	1.416	
	117520.656	117754	74.44	3d^4 6d^{5}D; ^{4}F	9.38	3d^4 6d^{5}D; ^{4}G	1.225	
		118774	99.41	3d^4 5s ^{1}F; ^{2}F	0.19	3d^4 5s ^{3}F; ^{4}F	1.144	
		119716	68.84	3d^4 4d ^{1}D; ^{2}F	18.21	3d^4 4d ^{1}D; ^{2}F	1.143	
		120271	72.88	3d^4 4d ^{1}D; ^{2}G	17.16	3d^4 4d ^{1}D; ^{2}G	0.889	
	121036.359	121037	96.08	3d^4 8s^{5}D; ^{6}D	3.74	3d^4 8s^{5}D; ^{4}D	1.583	
		121384	96.17	3d^4 8s ^{5}D; ^{4}D	3.73	3d^4 8s^{5}D; ^{6}D	1.435	
		121997	99.52	3d^4 6s ^{3}H; ^{4}H	0.15	3d^4 6s ^{3}G; ^{4}G	0.667	
		122153	97.47	3d^4 5d ^{3}H; ^{4}H	0.77	3d^4 6d ^{3}H; ^{4}H	0.669	
		122482	47.65	3d^4 4d ^{1}F; ^{2}F	45.69	3d^4 5d ^{3}H; ^{2}F	1.143	
		122805	78.67	3d^4 5d ^{3}H; ^{2}G	8.59	3d^4 4d ^{1}F; ^{2}G	0.896	
		123077	83.86	3d^4 5d ^{3}H; ^{4}F	4.07	3d^4 5d ^{3}G; ^{4}F	1.230	
		123109	75.96	3d^4 4d ^{1}F; ^{2}G	8.22	3d^4 5d ^{3}H; ^{2}G	0.889	
		123607	18.57	3d^4 5d ^{3}P; ^{4}F	17.16	3d^4 5d ^{3}H; ^{4}G	1.163	
		123628	44.91	3d^4 5d ^{3}H; ^{4}G	16.47	3d^4 5d ^{3}F; ^{4}G	1.050	
		123950	19.24	3d^4 5d ^{3}P; ^{4}F	15.68	3d^4 5d ^{3}H; ^{2}F	1.205	
	124310.148	124309	30.49	3d^4 9s^{5}D; ^{6}D	17.39	3d^4 6s ^{3}P; ^{4}D	1.445	
		124310	64.06	3d^4 9s ^{5}D; ^{6}D	8.2	3d^4 6s ^{3}P; ^{4}D	1.516	
4.5								
	12496.456	12467	99.87	3d^4 4s^{5}D; ^{6}D	0.04	3d^4 4s ^{3}F; ^{4}F	1.557	1.554
	20519.270	20545	98.97	3d^5^{4}G	0.39	3d^4 4s ^{3}G; ^{4}G	1.172	1.161
	30218.779	30239	99.19	3d^4 4s ^{3}H; ^{4}H	0.55	3d^4 4s ^{3}G; ^{4}G	0.971	0.978
	31219.336	31276	68.16	3d^4 4s ^{3}F; ^{4}F	18.87	3d^4 4s ^{3}F; ^{4}F	1.331	1.34
	32854.246	33014	84.12	3d^5^{4}F	7.86	3d^4 4s ^{3}F; ^{4}F	1.331	
	33618.941	33638	95.91	3d^4 4s ^{3}G; ^{4}G	1.61	3d^4 4s ^{3}F; ^{4}F	1.174	1.185
	34630.914	34627	68.03	3d^4 4s ^{3}H; ^{2}H	28.06	3d^5^{2}H	0.916	
	35610.305	35591	65.67	3d^5^{2}H	30.53	3d^4 4s ^{3}H; ^{2}H	0.914	
	36272.523	36264	73.45	3d^5^{2}G	14.67	3d^4 4s ^{3}G; ^{2}G	1.103	
	38563.008	38559	74.32	3d^4 4s ^{3}G; ^{2}G	12.32	3d^4 4s ^{1}G; ^{2}G	1.111	1.1
	39824.371	39778	47.56	3d^4 4s ^{1}G; ^{2}G	26.93	3d^4 4s ^{1}G; ^{2}G	1.111	
	52321.023	52196	92.1	3d^5^{2}G	4.46	3d^3 4s^2^{2}G	1.112	
	53923.523	53942	97.14	3d^3 4s^2^{4}F	1.92	3d^5^{4}F	1.333	
	54867.512	54842	77.26	3d^4 4s ^{3}F; ^{4}F	21.76	3d^4 4s ^{3}F; ^{4}F	1.334	
	62688.961	62579	64.55	3d^4 4s ^{1}G; ^{2}G	34.36	3d^4 4s ^{1}G; ^{2}G	1.112	
		66194	93.6	3d^3 4s^2^{2}G	4.4	3d^5^{2}G	1.109	
		69833	98	3d^3 4s^2^{2}H	1.22	3d^3 4s^2^{2}G	0.911	
	83240.422	83241	99.69	3d^4 5s^{5}D; ^{6}D	0.1	3d^4 4d^{5}D; ^{6}D	1.557	
	86847.008	86946	98.1	3d^4 4d^{5}D; ^{6}G	1.24	3d^4 4d^{5}D; ^{6}F	1.275	
	87687.508	87629	83.8	3d^4 4d^{5}D; ^{6}D	15.34	3d^4 4d^{5}D; ^{6}F	1.537	
	87948.531	87981	82.98	3d^4 4d^{5}D; ^{6}F	15.7	3d^4 4d^{5}D; ^{6}D	1.453	
	89325.281	89463	96.29	3d^4 4d^{5}D; ^{4}G	1.25	3d^4 4d ^{3}H; ^{4}G	1.173	
	90850.961	90940	95.03	3d^4 4d^{5}D; ^{4}F	1.24	3d^4 4d ^{3}H; ^{4}F	1.333	
	100135.781	100146	98.63	3d^4 5s ^{3}H; ^{4}H	0.55	3d^4 5s ^{3}G; ^{4}G	0.971	
	101021.797	101050	97.05	3d^4 5s ^{3}H; ^{2}H	1.03	3d^4 5s ^{3}F; ^{4}F	0.917	
	101382.938	101334	78.26	3d^4 5s ^{3}F; ^{4}F	18.49	3d^4 5s ^{3}F; ^{4}F	1.325	
	103627.039	103630	97.29	3d^4 5s ^{3}G; ^{4}G	1.08	3d^4 5s ^{3}F; ^{4}F	1.173	
	103755.383	103685	88.57	3d^4 4d ^{3}H; ^{4}I	6.31	3d^4 4d ^{3}H; ^{4}H	0.744	
	104023.961	103797	90.9	3d^4 4d ^{3}H; ^{4}H	6.16	3d^4 4d ^{3}H; ^{4}I	0.956	
		104192	65.91	3d^4 4d ^{3}H; ^{2}G	10.97	3d^4 4d ^{3}G; ^{2}G	1.137	
		104463	68.26	3d^4 4d ^{3}H; ^{4}F	10.15	3d^4 4d ^{3}H; ^{2}G	1.301	
	104666.359	104652	76.75	3d^4 4d ^{3}H; ^{4}G	11.59	3d^4 5d^{5}D; ^{4}G	1.174	
	105255.305	105089	97.43	3d^4 5s ^{3}G; ^{2}G	0.78	3d^4 4d ^{3}H; ^{2}G	1.111	
	105365.508	105269	75.66	3d^4 4d ^{3}H; ^{2}H	14.16	3d^4 4d ^{3}F; ^{2}H	0.913	
	105650.000	106045	46.53	3d^4 4d ^{3}F; ^{4}F	20.53	3d^4 4d ^{3}P; ^{4}F	1.330	
		106090	72.85	3d^4 4d ^{3}F; ^{4}H	18.33	3d^4 4d ^{3}F; ^{4}H	0.971	
	106148.734	106220	60.76	3d^4 4d ^{3}F; ^{4}G	17.57	3d^4 5d^{5}D; ^{4}G	1.165	
		106597	39.66	3d^4 4d ^{3}P; ^{4}F	27.51	3d^4 4d ^{3}F; ^{4}F	1.331	

Table 1 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
		107044	99.86	3d^4 6s ^{5}D; ^{6}D	0.08	3d^4 5s^{5}D; ^{6}D	1.557	
	107111.761	107122	88.73	3d^4 5d^{5}D; ^{6}G	7.94	3d^4 5d^{5}D; ^{6}F	1.287	
		107341	38.96	3d^4 4d ^{3}F; ^{2}G	11.14	3d^4 4d ^{3}F; ^{2}H	1.050	
	107455.484	107422	42.71	3d^4 5d^{5}D; ^{6}D	40.03	3d^4 5d^{5}D; ^{6}F	1.457	
	107632.227	107505	27.96	3d^4 4d ^{3}G; ^{4}G	14.75	3d^4 5d^{5}D; ^{4}G	1.084	
		107520	30.28	3d^4 4d ^{3}G; ^{4}G	13.78	3d^4 4d ^{3}F; ^{2}H	1.093	
		107584	40.51	3d^4 4d ^{3}G; ^{4}F	27.49	3d^4 5d^{5}D; ^{4}F	1.278	
	107696.273	107688	51.28	3d^4 5d^{5}D; ^{6}D	45.84	3d^4 5d^{5}D; ^{6}F	1.495	
	107706.742	107780	43.06	3d^4 4d ^{3}G; ^{4}H	34.58	3d^4 4d ^{3}G; ^{4}I	0.875	
	107922.453	107946	46.4	3d^4 4d ^{3}G; ^{4}I	36.9	3d^4 4d ^{3}G; ^{4}I	0.874	
		108814	66.1	3d^4 5s ^{1}G; ^{2}G	33.16	3d^4 5s ^{1}G; ^{2}G	1.112	
		109086	70.51	3d^4 4d ^{3}G; ^{2}H	10.57	3d^4 4d ^{1}I; ^{2}H	0.914	
		110491	38.59	3d^4 5d ^{5}D; ^{4}F	27.12	3d^4 4d ^{3}D; ^{4}F	1.329	
		110798	55.72	3d^4 4d ^{3}G; ^{2}G	9.09	3d^4 4d ^{1}G; ^{2}G	1.116	
		110967	26.14	3d^4 5d^{5}D; ^{4}G	23.35	3d^4 4d ^{3}G; ^{4}G	1.172	
		112684	37.26	3d^4 4d ^{3}D; ^{2}G	35.89	3d^4 4d ^{1}I; ^{2}G	1.142	
		112762	52.41	3d^4 4d ^{3}D; ^{4}F	9.05	3d^4 4d ^{3}G; ^{4}F	1.285	
		112797	54.49	3d^4 4d ^{1}I; ^{2}H	26.43	3d^4 4d ^{1}G; ^{2}H	0.917	
		112951	72.71	3d^4 4d ^{3}D; ^{4}G	7.12	3d^4 5d^{5}D; ^{4}G	1.183	
		114095	51	3d^4 4d ^{1}G; ^{2}G	28.48	3d^4 4d ^{1}G; ^{2}G	1.108	
		114853	31.18	3d^4 4d ^{1}G; ^{2}H	22.65	3d^4 4d ^{1}I; ^{2}H	0.940	
		114958	37.03	3d^4 4d ^{1}I; ^{2}G	36.52	3d^4 4d ^{3}D; ^{2}G	1.084	
	115788.281	115789	99.79	3d^4 7s^{5}D; ^{6}D	0.08	3d^4 8s^{5}D; ^{6}D	1.557	
	116388.859	116388	76.91	3d^4 6d^{5}D; ^{6}G	18.65	3d^4 6d^{5}D; ^{6}F	1.312	
	116601.500	116577	41.43	3d^4 6d^{5}D; ^{6}D	38.69	3d^4 6d^{5}D; ^{6}F	1.455	
	116831.570	116795	54.62	3d^4 6d^{5}D; ^{6}D	41.53	3d^4 6d^{5}D; ^{6}F	1.497	
	117141.492	117185	80.77	3d^4 6d^{5}D; ^{4}G	7.12	3d^4 6d^{5}D; ^{4}F	1.186	
	117488.422	117492	82.77	3d^4 6d^{5}D; ^{4}F	7.03	3d^4 6d^{5}D; ^{4}G	1.322	
		120264	74	3d^4 4d ^{1}D; ^{2}G	17.55	3d^4 4d ^{1}D; ^{2}G	1.112	
	121246.773	121247	99.78	3d^4 8s^{5}D; ^{6}D	0.08	3d^4 7s^{5}D; ^{6}D	1.557	
		122055	97.86	3d^4 6s ^{3}H; ^{4}H	1.68	3d^4 6s ^{3}H; ^{2}H	0.969	
		122136	87.3	3d^4 5d ^{3}H; ^{4}I	10.35	3d^4 5d ^{3}H; ^{4}H	0.754	
		122238	87.49	3d^4 5d ^{3}H; ^{4}H	10.31	3d^4 5d ^{3}H; ^{4}I	0.945	
		122473	97.76	3d^4 6s ^{3}H; ^{2}H	1.7	3d^4 6s ^{3}H; ^{4}H	0.911	
		122883	73.27	3d^4 5d ^{3}H; ^{2}G	7.6	3d^4 5d ^{3}H; ^{2}H	1.100	
		123112	50.62	3d^4 4d ^{1}F; ^{4}G	18.74	3d^4 5d ^{3}H; ^{4}F	1.121	
		123170	60.55	3d^4 5d ^{3}H; ^{4}F	23.47	3d^4 4d ^{1}F; ^{2}G	1.266	
		123226	40.51	3d^4 5d ^{3}H; ^{2}H	22.36	3d^4 4d ^{1}F; ^{2}H	0.977	
		123701	61.11	3d^4 5d ^{3}H; ^{4}G	23.54	3d^4 5d ^{3}F; ^{4}G	1.174	
		123999	59.93	3d^4 4d ^{1}F; ^{2}H	16.95	3d^4 5d ^{3}F; ^{2}H	0.910	
		124254	50.39	3d^4 5d ^{3}P; ^{4}F	33.72	3d^4 5d ^{3}P; ^{4}F	1.333	
		124417	76.67	3d^4 6s ^{3}F; ^{4}F	20.3	3d^4 6s ^{3}F; ^{4}F	1.330	
	124523.727	124517	74.3	3d^4 5d ^{3}F; ^{4}H	22.22	3d^4 5d ^{3}F; ^{4}H	0.967	
		124524	99.82	3d^4 9s ^{5}D; ^{6}D	0.07	3d^4 8s^{5}D; ^{6}D	1.557	
		124537	67.28	3d^4 5s ^{3}F; ^{4}F	15.53	3d^4 4d ^{3}F; ^{4}F	1.333	
		124791	63.6	3d^4 5d ^{3}F; ^{4}F	16.28	3d^4 5d ^{3}F; ^{4}F	1.328	
5.5	20512.098	20544	98.97	3d^5 ^{4}G	0.38	3d^4 4s ^{3}G; ^{4}G	1.273	1.278
	30143.246	30099	98.84	3d^5^{2}I	0.45	3d^5^{2}H	0.924	
	30298.471	30333	99.36	3d^4 4s ^{3}H; ^{4}H	0.48	3d^4 4s ^{3}G; ^{4}G	1.134	1.234
	33694.141	33721	97.57	3d^4 4s ^{3}G; ^{4}G	1.29	3d^4 4s ^{3}H; ^{2}H	1.270	1.276
	34812.930	34812	63	3d^4 4s ^{3}H; ^{2}H	34.55	3d^5^{2}H	1.093	
	35707.473	35700	62.95	3d^5^{2}H	35.34	3d^4 4s ^{3}H; ^{2}H	1.091	
	40228.293	40215	99.61	3d^4 4s ^{1}I; ^{2}I	0.23	3d^4 4s ^{3}H; ^{2}H	0.923	
		70068	99.26	3d^3 4s^2^{2}H	0.7	3d^5^{2}H	1.091	
	86980.078	87088	98.47	3d^4 4d^{5}D; ^{6}G	0.91	3d^4 4d^{5}D; ^{6}F	1.344	
	88001.336	88060	98.58	3d^4 4d^{5}D; ^{6}F	0.92	3d^4 4d^{5}D; ^{6}G	1.454	
	89508.499	89667	96.63	3d^4 4d^{5}D; ^{4}G	1.28	3d^4 4d ^{3}H; ^{4}G	1.274	
	100221.594	100240	98.9	3d^4 5s ^{3}H; ^{4}H	0.5	3d^4 5s ^{3}G; ^{4}G	1.134	
	101194.789	101240	98.94	3d^4 5s ^{3}H; ^{2}H	0.51	3d^4 5s ^{3}H; ^{4}H	1.092	
	103737.000	103746	98.84	3d^4 5s ^{3}G; ^{4}G	0.45	3d^4 5s ^{3}H; ^{4}H	1.272	
	103843.312	103775	85.39	3d^4 4d ^{3}H; ^{4}I	9.97	3d^4 4d ^{3}H; ^{4}H	0.983	
		103893	88.53	3d^4 4d ^{3}H; ^{4}H	9.56	3d^4 4d ^{3}H; ^{4}I	1.116	
	104460.164	104435	98.5	3d^4 4d ^{3}H; ^{4}K	0.33	3d^4 5d ^{3}H; ^{4}K	0.771	
	105423.344	105209	77.79	3d^4 4d ^{3}H; ^{4}G	10.85	3d^4 5d^{5}D; ^{4}G	1.273	
		105425	76.32	3d^4 4d ^{3}H; ^{2}H	15.39	3d^4 4d ^{3}F; ^{2}H	1.091	
	106145.227	105984	81.51	3d^4 4d ^{3}H; ^{2}I	6.61	3d^4 4d ^{1}I; ^{2}I	0.935	
		106161	73.86	3d^4 4d ^{3}F; ^{4}H	18.04	3d^4 4d ^{3}F; ^{4}H	1.125	
	106293.438	106326	60.79	3d^4 4d ^{3}F; ^{4}G	19.45	3d^4 5d^{5}D; ^{4}G	1.265	
	107246.797	107268	92.17	3d^4 5d^{5}D; ^{6}G	5.41	3d^4 5d^{5}D; ^{6}F	1.349	

Table 1 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
		107578	31.05	3d^4 4d ^{3}F; ^{2}H	21.96	3d^4 4d ^{3}G; ^{4}G	1.142	
	107701.281	107677	50.1	3d^4 5d^{5}D; ^{6}F	17.6	3d^4 4d ^{3}G; ^{4}G	1.330	
		107695	43.28	3d^4 5d ^{5}D; ^{6}F	26.81	3d^4 4d ^{3}G; ^{4}G	1.319	
	107760.703	107825	42.48	3d^4 4d ^{3}G; ^{4}I	36.99	3d^4 4d ^{3}G; ^{4}H	1.052	
	108017.984	108032	54.18	3d^4 4d ^{3}G; ^{4}H	35.98	3d^4 4d ^{3}G; ^{4}I	1.068	
		108761	80.93	3d^4 5s ^{1}I; ^{2}I	15.73	3d^4 4d ^{3}G; ^{2}I	0.924	
		108999	69.47	3d^4 4d ^{3}G; ^{2}I	18.77	3d^4 5s ^{1}I; ^{2}I	0.927	
		109210	70.55	3d^4 4d ^{3}G; ^{2}H	10.87	3d^4 4d ^{1}I; ^{2}H	1.090	
		110986	30.22	3d^4 5d^{5}D; ^{4}G	24.08	3d^4 4d ^{3}G; ^{4}G	1.273	
		112827	53.21	3d^4 4d ^{1}I; ^{2}H	28.34	3d^4 4d ^{1}G; ^{2}H	1.093	
		112941	77.45	3d^4 4d ^{3}D; ^{4}G	8.44	3d^4 5d^{5}D; ^{4}G	1.272	
		113274	44.92	3d^4 4d ^{1}G; ^{2}I	30.97	3d^4 4d ^{1}I; ^{2}I	0.924	
		114519	35.6	3d^4 4d ^{1}I; ^{2}I	15.66	3d^4 4d ^{1}G; ^{2}I	0.957	
		114940	28.91	3d^4 4d ^{1}G; ^{2}H	21.28	3d^4 4d ^{1}I; ^{2}H	1.058	
	116531.117	116523	86.34	3d^4 6d^{5}D; ^{6}G	12.18	3d^4 6d^{5}D; ^{6}F	1.357	
	116828.922	116783	86.77	3d^4 6d^{5}D; ^{6}F	12.31	3d^4 6d^{5}D; ^{6}G	1.441	
	117342.328	117368	88.08	3d^4 6d^{5}D; ^{4}G	4.58	3d^4 5d ^{3}H; ^{4}G	1.274	
		122134	98.35	3d^4 6s ^{3}H; ^{4}H	1.28	3d^4 6s ^{3}H; ^{2}H	1.133	
		122215	83.19	3d^4 5d ^{3}H; ^{4}I	13.6	3d^4 5d ^{3}H; ^{4}H	0.987	
6.5								
	30149.879	30124	99.28	3d^5^{2}I	0.26	3d^4 4d ^{3}H; ^{2}I	1.077	
	30391.832	30444	99.79	3d^4 4s ^{3}H; ^{4}H	0.08	3d^4 4s ^{1}I; ^{2}I	1.231	1.234
	40202.109	40209	99.78	3d^4 4s ^{1}I; ^{2}I	0.08	3d^4 4s ^{3}H; ^{4}H	1.077	
	87137.023	87258	99.38	3d^4 4d^{5}D; ^{6}G	0.45	3d^4 5d^{5}D; ^{6}G	1.385	
	100322.078	100355	99.77	3d^4 5s ^{3}H; ^{4}H	0.11	3d^4 5s ^{1}I; ^{2}I	1.231	
	103948.250	103887	83.68	3d^4 4d ^{3}H; ^{4}I	12.14	3d^4 4d ^{3}H; ^{4}H	1.123	
	104190.523	103993	86.46	3d^4 4d ^{3}H; ^{4}H	11.79	3d^4 4d ^{3}H; ^{4}I	1.216	
	104539.984	104521	97.82	3d^4 4d ^{3}H; ^{4}K	0.82	3d^4 4d ^{3}H; ^{2}K	0.965	
	105124.836	105151	97.95	3d^4 4d ^{3}H; ^{2}K	0.83	3d^4 4d ^{3}H; ^{4}K	0.935	
	106342.898	106180	71.17	3d^4 4d ^{3}H; ^{2}I	13.03	3d^4 4d ^{3}F; ^{4}H	1.104	
		106245	64.04	3d^4 4d ^{3}F; ^{4}H	15.12	3d^4 4d ^{3}F; ^{4}H	1.201	
	107412.031	107448	98.46	3d^4 5d^{5}D; ^{6}G	0.97	3d^4 7s^{5}D; ^{6}G	1.385	
	107846.664	107906	61.85	3d^4 4d ^{3}G; ^{4}I	35.41	3d^4 4d ^{3}G; ^{4}H	1.151	
	108103.953	108112	61.9	3d^4 4d ^{3}G; ^{4}H	32.03	3d^4 4d ^{3}G; ^{4}I	1.188	
		108784	94.85	3d^4 5s ^{1}I; ^{2}I	3.91	3d^4 4d ^{3}G; ^{2}I	1.077	
		109219	80.93	3d^4 4d ^{3}G; ^{2}I	10.65	3d^4 4d ^{1}I; ^{2}I	1.077	
		112233	99.34	3d^4 4d ^{1}I; ^{2}K	0.3	3d^4 5d ^{1}I; ^{2}K	0.934	
		113315	47.09	3d^4 4d ^{1}G; ^{2}I	27.69	3d^4 4d ^{1}I; ^{2}I	1.077	
		114562	46.34	3d^4 4d ^{1}I; ^{2}I	17.97	3d^4 4d ^{1}G; ^{2}I	1.077	
	116708.656	116695	98.86	3d^4 7s^{5}D; ^{6}G	1.01	3d^4 5d^{5}D; ^{6}G	1.385	
		122230	99.81	3d^4 6s ^{3}H; ^{4}H	0.1	3d^4 6s ^{1}I; ^{2}I	1.231	
7.5								
	104069.906	104028	96.31	3d^4 4d ^{3}H; ^{4}I	2.87	3d^4 4d ^{3}G; ^{4}I	1.200	
	104633.094	104624	98.23	3d^4 4d ^{3}H; ^{4}K	0.66	3d^4 4d ^{3}H; ^{2}K	1.091	
	105285.422	105337	98.8	3d^4 4d ^{3}H; ^{2}K	0.71	3d^4 4d ^{3}H; ^{4}K	1.067	
	107981.719	108065	95.95	3d^4 4d ^{3}G; ^{4}I	2.85	3d^4 4d ^{3}H; ^{4}I	1.200	
		112245	99.47	3d^4 4d ^{1}I; ^{2}K	0.3	3d^4 5d ^{1}I; ^{2}K	1.067	
		113013	99.56	3d^4 4d ^{1}I; ^{2}L	0.24	3d^4 5d ^{1}I; ^{2}L	0.941	
8.5								
	104734.508	104744	99.46	3d^4 4d ^{3}H; ^{4}K	0.33	3d^4 5d ^{3}H; ^{4}K	1.177	
		113033	99.58	3d^4 4d ^{1}I; ^{2}L	0.24	3d^4 5d ^{1}I; ^{2}L	1.059	

Table 2
Values of the intra-configuration fine structure parameters for Cr II even configurations.

Configuration	Parameter	Value (cm^{-1})
3d^5	E_{av}	34907(13)
	F^2(3d,3d)	54319(62)
	F^4(3d,3d)	31973(71)
	ζ_{3d}	199(23)
	α	52(1)
	β	−83(19)
3d^{4}4s	E_{av}	39185(8)
	F^2(3d,3d)	59200(40)
	F^4(3d,3d)	35099(61)
	G^2(3d,4s)	7044(27)
	ζ_{3d}	231(11)
	α	58(2)
	β	−125(23)
	T$_s$	21(9)
3d^{3}4s^2	E_{av}	68847(23)
	F^2(3d,3d)	63138(89)
	F^4(3d,3d)	37001(98)
	ζ_{3d}	257(21)
	α	21(2)
	β	0^f
3d^{4}5s	E_{av}	107550(11)
	F^2(3d,3d)	59996(59)
	F^4(3d,3d)	37827(69)
	G^2(3d,5s)	1448(30)
	ζ_{3d}	234^d
	α	65(2)
	β	0^f
	T$_s$	29(7)
3d^{4}6s	E_{av}	129035(20)
	F^2(3d,3d)	60565^d
	F^4(3d,3d)	37986^d
	G^2(3d,6s)	723(42)
	ζ_{3d}	235^d
	α	0^f
	β	0^f
3d^{4}7s	E_{av}	139030(21)
	F^2(3d,3d)	60583^d
	F^4(3d,3d)	38050^d
	G^2(3d,7s)	270^d
	ζ_{3d}	236^d
	α	0^f
	β	0^f
3d^{4}8s	E_{av}	144504(30)
	F^2(3d,3d)	60853^d
	F^4(3d,3d)	37500^d
	G^2(3d,8s)	148^d
	ζ_{3d}	236^d
	α	0^f
	β	0^f
3d^{4}9s	E_{av}	144523(43)
	F^2(3d,3d)	60853^d
	F^4(3d,3d)	37500^d
	G^2(3d,9s)	92^d
	ζ_{3d}	236^d
	α	0^f
	β	0^f
3d^{4}4d	E_{av}	112817(22)
	F^2(3d,3d)	59397(56)
	F^4(3d,3d)	40284(119)
	ζ_{3d}	244(11)
	ζ_{4d}	10^d
	α	46(2)

(*continued on next page*)

Table 2 (*continued*)

Configuration	Parameter	Value (cm^{-1})
	β	-52^d
	F^2(3d,4d)	4266(74)
	F^4(3d,4d)	1600(88)
	G^0(3d,4d)	1694(12)
	G^2(3d,4d)	1297(67)
	G^4(3d,4d)	619(67)
3d^{4}5d	E_{av}	131497(14)
	F^2(3d,3d)	60812^d
	F^4(3d,3d)	37673^d
	ζ_{3d}	244^d
	ζ_{5d}	4^d
	α	0^f
	β	0^f
	F^2(3d,5d)	1621^d
	F^4(3d,5d)	785^d
	G^0(3d,5d)	931^d
	G^2(3d,5d)	763^d
	G^4(3d,5d)	520^d
3d^{4}6d	E_{av}	140071(11)
	F^2(3d,3d)	60583^d
	F^4(3d,3d)	37500^d
	ζ_{3d}	244^d
	ζ_{6d}	2^d
	α	0^f
	β	0^f
	F^2(3d,6d)	799^d
	F^4(3d,6d)	354^d
	G^0(3d,6d)	403^d
	G^2(3d,6d)	383^d
	G^4(3d,6d)	267^d

^{f} Frozen to zero.
^{d} Deduced from *ab initio* or fs calculations.

Table 3
Values of even configuration interaction parameters.

Configurations	Parameter[a]	Value (cm^{-1})
$3d^5$–$3d^3 4s^2$	R^2	11076(194)
$3d^5$–$3d^4 4s$	R^2	−3710(55)
$3d^5$–$3d^4 5s$	R^2	−2799(450)
$3d^5$–$3d^4 4d$	R^2	9075(279)
	R^4	7754(354)
$3d^5$–$3d^4 5d$	R^2	3736(462)
	R^4	2445(480)
$3d^5$–$3d^4 6d$	R^2	2892(499)
	R^4	3168(700)
$3d^4 4s$–$3d^3 4s^2$	R^2	−897(350)
$3d^4 4s$–$3d^4 5s$	E^2	2911(478)
$3d^4 4s$–$3d^4 6s$	E^2	2053(500)
$3d^4 4s$–$3d^4 4d$	D^2	6514(266)
	E^2	2097(391)
$3d^4 4s$–$3d^4 5d$	D^2	2657(498)

[a] For meaning of R^2, D^2, E^2 and R^4 see Cowan's book [28].

Table 4
Proposals of new positions for the quartet 3d^4(^{5}D)5d ^{4}F.

J-value	Position given in [27] (cm^{-1})	Our proposed position (cm^{-1})
1.5	107516.711	110256
2.5	107726.773	110324
3.5	107850.552	110443
4.5	107947.996	110491

Table 5

Comparison of the experimental and calculated energy values, percentages of first and second components and g_J-factors for Cr II odd-parity configurations.

J-value	E_{obs} (cm⁻¹) [8,27]	E_{calc} (cm⁻¹)	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
0.5								
	46823.305	46811	99.48	3d⁴ 4p ⁵D; ⁶F	0.24	3d⁴ 5p ⁵D; ⁶F	−0.669	−0.689
	48749.277	48685	79.02	3d⁴ 4p ⁵D; ⁴P	18.02	3d⁴ 4p⁵D; ⁶D	2.790	2.844
	49492.711	49455	81.70	3d⁴ 4p⁵D; ⁶D	17.72	3d⁴ 4p⁵D; ⁴P	3.217	3.155
	54417.957	54369	97.15	3d⁴ 4p⁵D; ⁴D	0.89	3d⁴ 4p ³P; ⁴D	−0.002	0.007
	63801.754	63839	48.15	3d⁴ 4p ³P; ²S	42.74	3d⁴ 4p ³P; ²S	1.951	
	65029.336	64748	48.95	3d⁴ 4p ³P; ⁴D	34.21	3d⁴ 4p ³P; ⁴D	0.021	
	66256.438	66425	52.96	3d⁴ 4p ³P; ⁴P	34.21	3d⁴ 4p ³P; ⁴P	2.540	2.545
	66871.828	66711	53.48	3d⁴ 4p ³P; ²P	27.84	3d⁴ 4p ³P; ²P	0.819	
	67859.562	68024	65.08	3d⁴ 4p ³F; ⁴D	19.78	3d⁴ 4p ³F; ⁴D	0.003	
	73406.891	73552	95.14	3d⁴ 4p ³D; ⁴D	1.05	3d⁴ 4p ³D; ²P	0.016	
	74920.383	74592	93.54	3d⁴ 4p ³D; ⁴P	3.65	3d⁴ 4p ³P; ⁴P	2.622	
	74853.852	74836	50.96	3d⁴ 4p ³D; ²P	32.63	3d⁴ 4p ¹S; ²P	0.697	
	77777.320	77681	36.24	3d⁴ 4p ¹S; ²P	34.51	3d⁴ 4p ³D; ²P	0.666	
	81648.641	81602	95.09	3d³ 4s 4p ⁴F.³P; ⁶D	2.28	3d³ 4s 4p ⁴P. ³P; ⁶D	3.258	
	81734.648	81733	97.20	3d³ 4s 4p ⁴F.³P; ⁶F	1.87	3d³ 4s 4p ⁴F. ³P; ⁶D	−0.589	
	82853.891	82762	68.50	3d⁴ 4p ¹D; ²P	15.36	3d⁴ 4p ¹D; ²P	0.667	
	85486.164	85333	89.00	3d³ 4s 4p ⁴F.³P; ⁴D	4.67	3d³ 4s 4p ⁴P. ³P; ⁴D	−0.003	
	89507.961	89576	58.41	3d⁴ 4p ³P; ⁴P	32.60	3d⁴ 4p ³P; ⁴P	2.651	
	90475.375	90549	35.99	3d⁴ 4p ³P; ⁴D	25.63	3d⁴ 4p ³F; ⁴D	0.015	
	92988.815	92943	98.10	3d⁴ 5p⁵D; ⁶F	1.11	3d⁴ 5p⁵D; ⁴D	−0.660	
		93314	52.28	3d⁴ 5p ⁵D; ⁶D	30.55	3d⁴ 5p⁵D; ⁴P	3.123	
		93675	64.65	3d³ 4s 4p ⁴P.³P; ⁶D	31.97	3d⁴ 5p⁵D; ⁴P	3.099	
	93800.484	93815	44.02	3d⁴ 4p ³F; ⁴D	19.83	3d⁴ 4p ³P; ⁴D	0.033	
	93968.672	93931	46.54	3d⁴ 5p⁵D; ⁶D	34.56	3d⁴ 5p⁵D; ⁴P	3.065	
	94624.703	94640	54.50	3d⁴ 4p ³P; ²P	27.05	3d⁴ 4p ³P; ²P	0.642	
	94839.211	94764	82.72	3d⁴ 5p⁵D; ⁴D	4.46	3d³ 4s 4p ⁴F. ¹P; ⁴D	0.039	
		96711	51.34	3d⁴ 4p ³P; ²S	45.84	3d⁴ 4p ³P; ²S	1.998	
	97168.469	97369	78.91	3d³ 4s 4p ⁴P.³P; ⁴P	8.30	3d³ 4s 4p ²D. ³P; ⁴P	2.660	
		100156	58.83	3d³ 4s 4p ²P.³P; ⁴P	24.24	3d³ 4s 4p ²D. ³P; ⁴P	2.623	
		100322	47.95	3d³ 4s 4p ²P.³P; ⁴D	32.52	3d³ 4s 4p ⁴P. ³P; ⁴D	0.068	
		101245	52.53	3d³ 4s 4p ⁴P.³P; ²P	31.21	3d³ 4s 4p ²P. ³P; ²S	1.086	
		101966	62.97	3d³ 4s 4p ²P.³P; ²S	28.29	3d³ 4s 4p ⁴P. ³P; ²P	1.560	
	102619.641	102797	54.42	3d³ 4s 4p ⁴P.³P; ⁴D	37.35	3d³ 4s 4p ²P. ³P; ⁴D	0.013	
		103756	39.64	3d³ 4s 4p ⁴F.¹P; ⁴D	34.28	3d³ 4s 4p ²D. ³P; ⁴D	0.009	
	104439.570	104463	39.26	3d³ 4s 4p ²D.³P; ⁴D	32.51	3d³ 4s 4p ⁴F. ¹P; ⁴D	0.020	
		105121	45.07	3d³ 4s 4p ²D.³P; ²P	22.25	3d³ 4s 4p ²P. ³P; ²P	0.778	
	105392.508	105364	52.97	3d⁴ 4f⁵D; ⁴P	23.77	3d⁴ 4f⁵D; ⁶D	2.145	
		105482	56.32	3d⁴ 4f⁵D; ⁶F	33.06	3d⁴ 4f⁵D; ⁴P	0.848	
		105524	58.02	3d⁴ 4f⁵D; ⁶D	26.65	3d⁴ 4f⁵D; ⁴D	1.888	
		105585	38.48	3d³ 4s 4p ²D.³P; ⁴P	32.64	3d³ 4s 4p ²P. ³P; ⁴P	2.526	
		105650	58.48	3d⁴ 4f⁵D; ⁴D	19.59	3d⁴ 4f⁵D; ⁶F	0.457	
1.5								
	46905.137	46882	99.49	3d⁴ 4p ⁵D; ⁶F	0.24	3d⁴ 5p ⁵D; ⁶F	1.067	1.124
	48398.871	48337	96.69	3d⁴ 4p⁵D; ⁶P	2.71	3d⁴ 4p⁵D; ⁴P	2.383	2.382
	49005.848	48920	73.32	3d⁴ 4p⁵D; ⁴P	21.01	3d⁴ 4p⁵D; ⁶D	1.783	1.802
	49564.504	49510	78.38	3d⁴ 4p⁵D; ⁶D	20.85	3d⁴ 4p⁵D; ⁴P	1.840	1.824
	51584.102	51804	95.62	3d⁴ 4p⁵D; ⁴F	1.87	3d⁴ 4p ³F; ⁴F	0.400	0.406
	54499.492	54443	97.13	3d⁴ 4p⁵D; ⁴D	0.84	3d⁴ 4p ³P; ⁴D	1.200	1.178
	64061.680	64058	48.93	3d⁴ 4p ³P; ⁴D	34.22	3d⁴ 4p ³P; ⁴D	1.202	1.199
	66354.758	66555	51.57	3d⁴ 4p ³P; ⁴P	33.21	3d⁴ 4p ³P; ⁴P	1.676	1.671
	66649.391	66747	25.19	3d⁴ 4p ³P; ²P	21.91	3d⁴ 4p ³F; ²D	1.078	
	67070.445	66973	62.84	3d⁴ 4p ³F; ⁴F	12.56	3d⁴ 4p ³F; ⁴F	0.500	
	67379.297	67382	31.57	3d⁴ 4p ³P; ²P	17.16	3d⁴ 4p ³F; ²D	1.035	
	67870.211	68035	63.02	3d⁴ 4p ³F; ⁴D	18.94	3d⁴ 4p ³F; ⁴D	1.195	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	68305.555	68164	52.07	3d^4 4p ^{3}P; ^{4}S	42.86	3d^4 4p ^{3}P; ^{4}S	1.974	1.978
	69348.141	69473	35.24	3d^4 4p ^{3}G; ^{4}F	27.20	3d^4 4p ^{3}P; ^{2}D	0.637	
	69638.594	69743	50.57	3d^4 4p ^{3}G; ^{4}F	17.92	3d^4 4p ^{3}P; ^{2}D	0.571	
	73411.883	73558	93.22	3d^4 4p ^{3}D; ^{4}F	1.38	3d^4 4p ^{3}D; ^{4}F	1.194	
	74273.336	74293	85.27	3d^4 4p ^{3}D; ^{4}F	10.95	3d^4 4p ^{3}G; ^{4}F	0.422	
	74717.555	74466	91.95	3d^4 4p ^{3}D; ^{4}P	3.48	3d^4 4p ^{3}P; ^{4}P	1.712	
	74984.695	74905	56.44	3d^4 4p ^{3}D; ^{2}P	28.91	3d^4 4p ^{1}S; ^{2}P	1.341	
	77713.273	77640	37.11	3d^4 4p ^{1}S; ^{2}P	24.02	3d^4 4p ^{3}D; ^{2}P	1.288	
	78109.453	78086	75.78	3d^4 4p ^{3}D; ^{2}D	6.18	3d^4 4p ^{3}F; ^{2}D	0.843	
		78961	99.78	3d^3 4s 4p ^{4}F.^{3}P; ^{6}G	0.08	3d^3 4s 4p ^{4}F. ^{3}P; ^{4}F	−0.002	
	80288.023	80280	61.84	3d^4 4p ^{1}D; ^{2}D	19.83	3d^4 4p ^{1}D; ^{2}D	0.804	
	81707.328	81687	92.04	3d^3 4s 4p ^{4}F.^{3}P; ^{6}F	6.91	3d^3 4s 4p ^{4}F. ^{3}P; ^{6}D	1.125	
	81824.070	81812	89.89	3d^3 4s 4p ^{4}F.^{3}P; ^{6}D	7.26	3d^3 4s 4p ^{4}F. ^{3}P; ^{6}F	1.809	
	82919.914	82818	66.51	3d^4 4p ^{1}D; ^{2}P	14.78	3d^4 4p ^{1}D; ^{2}P	1.333	
	85586.523	85443	88.24	3d^3 4s 4p ^{4}F.^{3}P; ^{4}D	4.61	3d^3 4s 4p ^{4}P. ^{3}P; ^{4}D	1.198	
	86919.008	86710	70.85	3d^4 4p ^{1}F; ^{2}D	9.55	3d^4 4p ^{3}P; ^{2}D	0.798	
	87628.734	87802	67.02	3d^3 4s 4p ^{4}F.^{3}P; ^{4}F	15.19	3d^3 4s 4p ^{4}F. ^{3}P; ^{2}D	0.476	
	88604.250	88431	69.92	3d^3 4s 4p ^{4}F.^{3}P; ^{2}D	12.75	3d^3 4s 4p ^{4}F. ^{3}P; ^{4}F	0.726	
	89422.328	89500	56.63	3d^4 4p ^{3}P; ^{4}P	31.52	3d^4 4p ^{3}P; ^{4}P	1.727	
	90262.125	90005	66.11	3d^4 4p ^{3}F; ^{4}F	16.27	3d^3 4s 4p ^{4}F. ^{3}P; ^{4}F	0.411	
	90450.617	90508	34.42	3d^4 4p ^{3}P; ^{4}D	24.46	3d^4 4p ^{3}F; ^{4}D	1.193	
	91556.359	91585	31.27	3d^4 4p ^{3}P; ^{2}D	23.25	3d^4 4p ^{3}P; ^{2}D	0.809	
	92234.906	92323	50.02	3d^4 4p ^{3}P; ^{4}S	40.61	3d^4 4p ^{3}P; ^{4}S	2.018	
	92612.203	92395	68.75	3d^3 4s 4p ^{4}P.^{3}P; ^{6}P	25.15	3d^4 5p^{5}D; ^{6}P	2.378	
	93047.287	93017	98.05	3d^4 5p^{5}D; ^{6}F	0.95	3d^4 5p^{5}D; ^{4}D	1.067	
	93574.430	93441	56.09	3d^4 5p^{5}D; ^{6}D	19.77	3d^4 5p^{5}D; ^{4}P	1.850	
	93740.241	93758	31.46	3d^3 4s 4p ^{4}P.^{3}P; ^{6}D	22.92	3d^4 5p^{5}D; ^{4}P	1.800	
	93769.992	93785	35.86	3d^4 4p ^{3}F; ^{4}D	15.00	3d^4 4p ^{3}P; ^{4}D	1.372	
	94002.493	93876	41.40	3d^4 5p^{5}D; ^{6}P	27.35	3d^3 4s 4p ^{4}P. ^{3}P; ^{6}D	2.158	
	94098.172	94045	45.93	3d^4 5p^{5}D; ^{4}P	26.20	3d^4 5p^{5}D; ^{6}D	1.870	
	94255.977	94331	94.33	3d^4 5p^{5}D; ^{4}F	1.86	3d^4 5p^{5}D; ^{4}D	0.433	
	94383.156	94425	57.55	3d^4 4p ^{3}P; ^{2}P	28.69	3d^4 4p ^{3}P; ^{2}P	1.332	
	94932.942	94856	83.91	3d^4 5p^{5}D; ^{4}D	4.55	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}D	1.192	
	97294.047	97472	80.74	3d^3 4s 4p ^{4}P.^{3}P; ^{4}P	7.18	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}P	1.734	
	98314.984	98100	50.46	3d^4 4p ^{3}F; ^{2}D	18.84	3d^4 4p ^{3}F; ^{2}D	0.800	
	98578.555	98816	77.09	3d^3 4s 4p ^{2}G.^{3}P; ^{4}F	12.35	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}F	0.402	
		100299	54.31	3d^3 4s 4p ^{2}P.^{3}P; ^{4}P	25.80	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}P	1.724	
	100691.820	100517	46.25	3d^3 4s 4p ^{2}P.^{3}P; ^{4}D	32.53	3d^3 4s 4p ^{4}P. ^{3}P; ^{4}D	1.191	
	101157.773	101417	77.12	3d^3 4s 4p ^{4}P.^{3}P; ^{2}P	4.19	3d^3 4s 4p ^{2}P. ^{3}P; ^{4}D	1.310	
	101986.992	102009	42.45	3d^3 4s 4p ^{2}D.^{3}P; ^{4}F	17.84	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}F	0.478	
	102602.312	102485	84.44	3d^3 4s 4p ^{2}P.^{3}P; ^{4}S	9.86	3d^4 4p ^{4}P. ^{3}P; ^{4}S	1.986	
	102684.391	102787	48.06	3d^3 4s 4p ^{4}P.^{3}P; ^{4}D	35.99	3d^3 4s 4p ^{2}P. ^{3}P; ^{4}D	1.176	
		103184	43.21	3d^3 4s 4p ^{2}P.^{3}P; ^{2}D	21.36	3d^3 4s 4p ^{2}D. ^{3}P; ^{2}D	0.798	
	104274.570	103907	37.61	3d^3 4s 4p ^{2}D.^{3}P; ^{4}D	35.39	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}D	1.203	
	104616.250	104559	32.41	3d^3 4s 4p ^{4}F.^{1}P; ^{4}D	30.33	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}D	1.220	
		104751	43.06	3d^3 4s 4p ^{2}D.^{3}P; ^{2}P	17.77	3d^3 4s 4p ^{2}D. ^{3}P; ^{2}P	1.335	
		104988	45.78	3d^3 4s 4p ^{4}F.^{1}P; ^{4}F	35.05	3d^4 4f^{5}D; ^{4}F	0.420	
	105283.430	105256	62.24	3d^4 4f^{5}D; ^{4}P	13.40	3d^4 4f^{5}D; ^{6}D	1.657	
		105386	29.87	3d^4 4f^{5}D; ^{6}D	25.81	3d^4 4f^{5}D; ^{6}F	1.404	
		105447	49.77	3d^4 4f^{5}D; ^{6}G	19.88	3d^4 4f^{5}D; ^{6}P	0.922	

Table 5 (continued)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
		105480	35.30	$3d^3\,4s\,4p\ ^2D.^3P;\ ^4P$	30.83	$3d^3\,4s\,4p\ ^2P.\ ^3P;\ ^4P$	1.716	
		105544	31.72	$3d^4\,4f\,^5D;\ ^6G$	30.42	$3d^4\,4f\,^5D;\ ^6F$	1.086	
		105629	39.25	$3d^4\,4f\,^5D;\ ^4D$	33.71	$3d^4\,4f\,^5D;\ ^6P$	1.698	
		105676	30.07	$3d^4\,4f\,^5D;\ ^6F$	28.22	$3d^4\,4f\,^5D;\ ^6D$	1.437	
		105946	60.12	$3d^4\,4f\,^5D;\ ^4F$	23.78	$3d^3\,4s\,4p\ ^4F.\ ^1P;\ ^4F$	0.463	
	106726.086	106544	81.23	$3d^3\,4s\,4p\ ^4P.^3P;\ ^4S$	10.67	$3d^3\,4s\,4p\ ^2P.\ ^3P;\ ^4S$	1.979	
	107212.344	106852	85.12	$3d^3\,4s\,4p\ ^4P.^3P;\ ^2D$	4.89	$3d^3\,4s\,4p\ ^4F.\ ^3P;\ ^2D$	0.812	
		109178	71.68	$3d^3\,4s\,4p\ ^2P.^3P;\ ^2P$	14.16	$3d^3\,4s\,4p\ ^2D.\ ^3P;\ ^2P$	1.328	
		109515	94.76	$3d^4\,6p\,^5D;\ ^6F$	1.85	$3d^4\,6p\,^5D;\ ^4P$	1.086	
	109661.352	109563	54.47	$3d^4\,6p\,^5D;\ ^4P$	24.54	$3d^4\,6p\,^5D;\ ^6D$	1.835	
		109880	73.59	$3d^4\,6p\,^5D;\ ^6P$	25.12	$3d^4\,6p\,^5D;\ ^6D$	2.259	
		110039	49.36	$3d^4\,6p\,^5D;\ ^6D$	32.09	$3d^4\,6p\,^5D;\ ^4P$	1.872	
	109914.492	110147	42.42	$3d^3\,4s\,4p\ ^2D.^3P;\ ^2D$	37.87	$3d^3\,4s\,4p\ ^2P.\ ^3P;\ ^2D$	0.803	
		110316	90.13	$3d^4\,6p\,^5D;\ ^4F$	2.39	$3d^3\,4s\,4p\ ^4F.\ ^1P;\ ^4F$	0.440	
		110435	48.04	$3d^4\,5p\,^3P;\ ^4D$	32.95	$3d^4\,5p\,^3P;\ ^4D$	1.205	
		110895	22.35	$3d^4\,5p\,^3P;\ ^4P$	15.70	$3d^4\,5p\,^3P;\ ^2P$	1.559	
	110931.633	111052	83.18	$3d^4\,6p\,^5D;\ ^4D$	4.91	$3d^3\,4s\,4p\ ^4F.\ ^1P;\ ^4D$	1.221	
		111231	27.52	$3d^4\,5p\,^3P;\ ^4P$	20.50	$3d^4\,5p\,^3P;\ ^2P$	1.493	
		111567	32.53	$3d^4\,5p\,^3P;\ ^4S$	23.47	$3d^4\,5p\,^3P;\ ^2D$	1.500	
		111731	32.78	$3d^4\,5p\,^3F;\ ^4F$	27.88	$3d^4\,5p\,^3F;\ ^2D$	0.719	
		111811	23.33	$3d^4\,4p\,^1D;\ ^2P$	17.24	$3d^4\,5p\,^3P;\ ^2D$	1.191	
		111980	42.68	$3d^4\,4p\,^1D;\ ^2P$	11.86	$3d^4\,4p\,^1D;\ ^2P$	1.311	
		112158	43.03	$3d^4\,5p\,^3F;\ ^4D$	20.74	$3d^4\,5p\,^3F;\ ^4F$	0.949	
		112229	36.20	$3d^4\,5p\,^3F;\ ^2D$	18.95	$3d^4\,5p\,^3F;\ ^4D$	0.826	
		114106	55.25	$3d^4\,5p\,^3G;\ ^4F$	39.84	$3d^3\,4s\,4p\ ^2F.\ ^3P;\ ^4F$	0.404	
		115080	52.69	$3d^3\,4s\,4p\ ^2F.^3P;\ ^4F$	33.60	$3d^4\,5p\,^3G;\ ^4F$	0.416	
		115176	58.22	$3d^4\,5f\,^5D;\ ^4P$	20.25	$3d^3\,4s\,4p\ ^4P.\ ^1P;\ ^4P$	1.642	
		115381	42.68	$3d^4\,5f\,^5D;\ ^6G$	34.01	$3d^4\,4p\,^5D;\ ^6F$	0.736	
	115430.875	115456	40.96	$3d^4\,5f\,^5D;\ ^6D$	19.62	$3d^4\,4p\,^5D;\ ^6G$	1.249	
		115505	46.29	$3d^4\,5f\,^5D;\ ^4D$	30.34	$3d^4\,4p\,^5D;\ ^6G$	0.831	
	115605.898	115599	33.31	$3d^4\,5f\,^5D;\ ^6F$	18.25	$3d^4\,5f\,^5D;\ ^6P$	1.259	
		115610	58.66	$3d^4\,4p\,^1D;\ ^2D$	20.26	$3d^4\,4p\,^1D;\ ^2D$	0.888	
		115721	54.40	$3d^4\,5f\,^5D;\ ^4F$	21.75	$3d^4\,4p\,^5D;\ ^4D$	0.742	
	115747.539	115750	61.71	$3d^4\,5f\,^5D;\ ^6P$	28.72	$3d^4\,4p\,^5D;\ ^6D$	2.112	
	115966.555	116200	55.52	$3d^3\,4s\,4p\ ^4P.^1P;\ ^4P$	32.24	$3d^4\,5f\,^5D;\ ^4P$	1.727	
		117167	48.18	$3d^3\,4s\,4p\ ^2F.^3P;\ ^4D$	36.50	$3d^3\,4s\,4p\ ^4P.\ ^1P;\ ^4D$	1.201	
	118622.562	118792	44.64	$3d^3\,4s\,4p\ ^4P.^1P;\ ^4D$	44.36	$3d^3\,4s\,4p\ ^2F.\ ^3P;\ ^4D$	1.199	
		120098	50.78	$3d^3\,4s\,4p\ ^2F.^3P;\ ^2D$	14.72	$3d^4\,5p\,^3D;\ ^2D$	0.795	
		120332	73.28	$3d^4\,5p\,^3D;\ ^4F$	11.76	$3d^4\,5p\,^3D;\ ^4D$	0.573	
		120470	42.18	$3d^4\,5p\,^3D;\ ^4D$	19.45	$3d^4\,5p\,^3D;\ ^2P$	1.132	
		120632	32.37	$3d^4\,5p\,^3D;\ ^2D$	13.39	$3d^3\,4s\,4p\ ^2F.\ ^3P;\ ^2D$	0.905	
		120834	50.01	$3d^4\,5p\,^3D;\ ^2P$	24.39	$3d^4\,5p\,^3D;\ ^4D$	1.268	
		120901	24.09	$3d^3\,4s\,4p\ ^2P.^1P;\ ^2P$	16.83	$3d^3\,4s\,4p\ ^2D.\ ^1P;\ ^2P$	1.179	
		120944	84.33	$3d^4\,4f\,^3H;\ ^4F$	3.80	$3d^4\,4f\,^3H;\ ^2D$	0.499	
2.5								
	47040.273	47001	99.51	$3d^4\,4p\,^5D;\ ^6F$	0.24	$3d^4\,5p\,^5D;\ ^6F$	1.315	1.314
	48491.059	48423	97.41	$3d^4\,4p\,^5D;\ ^6P$	2.08	$3d^4\,4p\,^5D;\ ^4P$	1.881	1.875
	49351.734	49267	66.85	$3d^4\,4p\,^5D;\ ^6D$	31.86	$3d^4\,4p\,^5D;\ ^4P$	1.640	1.628
	49706.262	49603	63.07	$3d^4\,4p\,^5D;\ ^4P$	32.55	$3d^4\,4p\,^5D;\ ^6D$	1.626	
	51669.406	51876	95.51	$3d^4\,4p\,^5D;\ ^4F$	1.84	$3d^4\,4p\,^3F;\ ^4F$	1.030	1.025
	54625.594	54559	97.13	$3d^4\,4p\,^5D;\ ^4D$	0.83	$3d^4\,4p\,^3D;\ ^4D$	1.372	1.376
	64448.750	64387	47.68	$3d^4\,4p\,^3P;\ ^4D$	33.40	$3d^4\,4p\,^3P;\ ^4D$	1.372	1.38
	65156.492	65273	51.44	$3d^4\,4p\,^3F;\ ^4G$	21.25	$3d^4\,4p\,^3F;\ ^4G$	0.573	0.593
	66726.781	66895	44.25	$3d^4\,4p\,^3P;\ ^4P$	28.34	$3d^4\,4p\,^3P;\ ^4P$	1.505	1.502
	67012.078	67104	30.66	$3d^4\,4p\,^3F;\ ^2D$	16.39	$3d^4\,4p\,^3F;\ ^4F$	1.238	
	67344.008	67317	74.02	$3d^4\,4p\,^3H;\ ^4G$	15.30	$3d^4\,4p\,^3F;\ ^4G$	0.584	
	67387.094	67397	60.33	$3d^4\,4p\,^3F;\ ^4F$	11.91	$3d^4\,4p\,^3F;\ ^4F$	1.073	
	67867.789	68034	57.32	$3d^4\,4p\,^3F;\ ^4D$	16.86	$3d^4\,4p\,^3F;\ ^4D$	1.337	
	68583.305	68542	32.72	$3d^4\,4p\,^3F;\ ^2F$	30.46	$3d^4\,4p\,^3G;\ ^2F$	0.881	
	69954.055	69604	43.26	$3d^4\,4p\,^3P;\ ^2D$	30.51	$3d^4\,4p\,^3P;\ ^2D$	1.186	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	69477.898	69998	76.94	3d^4 4p ^{3}G; ^{4}F	9.44	3d^4 4p ^{3}D; ^{4}F	1.023	
	70316.820	70219	71.08	3d^4 4p ^{3}G; ^{4}G	12.58	3d^4 4p ^{3}H; ^{4}G	0.600	
	70584.391	70448	45.01	3d^4 4p ^{3}G; ^{2}F	35.96	3d^4 4p ^{3}F; ^{2}F	0.856	
	73436.125	73577	91.46	3d^4 4p ^{3}D; ^{4}P	2.54	3d^4 4p ^{3}D; ^{4}F	1.365	
	74318.844	74248	84.13	3d^4 4p ^{3}D; ^{4}P	6.59	3d^4 4p ^{3}D; ^{4}F	1.529	
	74436.117	74294	35.72	3d^4 4p ^{1}G; ^{2}F	17.07	3d^4 4p ^{1}G; ^{2}F	0.961	
	74483.906	74383	61.59	3d^4 4p ^{3}D; ^{4}F	14.51	3d^4 4p ^{1}G; ^{2}F	1.003	
	76987.672	76938	72.72	3d^4 4p ^{3}D; ^{2}F	7.82	3d^4 4p ^{3}G; ^{2}F	0.858	
	77935.203	77905	77.02	3d^4 4p ^{3}D; ^{2}D	9.53	3d^4 4p ^{1}D; ^{2}D	1.201	
		79115	99.82	3d^3 4s 4p ^{4}F.^{3}P; ^{6}G	0.06	3d^3 4s 4p ^{4}F. ^{3}P; ^{4}F	0.857	
	80420.164	80431	58.30	3d^4 4p ^{1}D; ^{2}D	18.42	3d^4 4p ^{1}D; ^{2}D	1.195	
	81232.883	81189	68.03	3d^4 4p ^{1}D; ^{2}F	17.83	3d^4 4p ^{1}D; ^{2}F	0.862	
	81815.883	81830	82.80	3d^3 4s 4p ^{4}F.^{3}P; ^{6}D	14.47	3d^3 4s 4p ^{4}F. ^{3}P; ^{6}F	1.608	
	81961.867	81943	84.98	3d^3 4s 4p ^{4}F.^{3}P; ^{6}F	13.85	3d^3 4s 4p ^{4}F. ^{3}P; ^{6}D	1.364	
	84604.641	84394	87.93	3d^4 4p ^{1}F; ^{2}F	3.20	3d^4 4p ^{3}D; ^{2}F	0.859	
	85778.656	85652	88.04	3d^3 4s 4p ^{4}F.^{3}P; ^{4}D	4.58	3d^3 4s 4p ^{4}P. ^{3}P; ^{4}D	1.371	
	86507.328	86353	70.78	3d^4 4p ^{1}F; ^{2}D	10.06	3d^4 4p ^{3}P; ^{2}D	1.199	
	86566.461	86669	93.63	3d^3 4s 4p ^{4}F.^{3}P; ^{4}G	3.77	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}G	0.572	
	87766.594	88023	76.52	3d^3 4s 4p ^{4}F.^{3}P; ^{4}F	14.84	3d^4 4p ^{3}F; ^{4}F	1.034	
	89164.516	88910	82.10	3d^3 4s 4p ^{4}F.^{3}P; ^{2}D	5.55	3d^3 4s 4p ^{4}P. ^{3}P; ^{2}D	1.195	
	89453.031	89518	56.85	3d^4 4p ^{3}P; ^{4}P	31.61	3d^4 4p ^{3}P; ^{4}P	1.593	
	90258.195	90035	32.25	3d^4 4p ^{3}P; ^{4}D	23.01	3d^4 4p ^{3}F; ^{4}D	1.356	
	90441.766	90447	62.75	3d^4 4p ^{3}F; ^{4}F	17.68	3d^3 4s 4p ^{4}F. ^{3}P; ^{4}F	1.041	
	90706.805	91017	36.96	3d^4 4p ^{3}F; ^{2}F	21.60	3d^4 4p ^{3}F; ^{4}G	0.774	
	91078.711	91269	50.75	3d^4 4p ^{3}F; ^{4}G	16.95	3d^4 4p ^{3}F; ^{4}G	0.660	
	91426.047	91441	31.30	3d^4 4p ^{3}P; ^{2}D	23.62	3d^4 4p ^{3}P; ^{2}D	1.208	
	92417.891	92542	70.50	3d^3 4s 4p ^{4}P.^{3}P; ^{6}P	28.60	3d^4 5p^{5}D; ^{6}P	1.886	
		93138	45.29	3d^4 5p^{5}D; ^{6}F	37.27	3d^3 4s 4p ^{4}F. ^{3}P; ^{2}F	1.069	
	93143.853	93143	52.72	3d^4 5p^{5}D; ^{6}F	32.10	3d^3 4s 4p ^{4}F. ^{3}P; ^{2}F	1.103	
	93670.984	93624	43.33	3d^4 4p ^{3}F; ^{4}D	19.23	3d^4 4p ^{3}P; ^{4}D	1.380	
	93776.125	93709	61.24	3d^4 5p^{5}D; ^{6}D	23.84	3d^3 4s 4p ^{4}P. ^{3}P; ^{6}D	1.650	
	93973.992	93909	44.72	3d^4 5p^{5}D; ^{6}P	21.54	3d^3 4s 4p ^{4}P. ^{3}P; ^{6}P		
	94144.430	94027	58.32	3d^3 4s 4p ^{4}P.^{3}P; ^{6}D	26.19	3d^4 5p^{5}D; ^{6}D	1.679	
	94265.930	94246	64.23	3d^4 5p^{5}D; ^{4}P	15.20	3d^4 5p^{5}D; ^{6}P	1.627	
	94365.203	94407	87.99	3d^4 5p^{5}D; ^{4}F	4.40	3d^4 5p^{5}D; ^{4}P	1.081	
	95076.719	94993	82.35	3d^4 5p^{5}D; ^{4}D	4.41	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}D	1.368	
	97070.938	97285	84.37	3d^3 4s 4p ^{2}G.^{3}P; ^{4}G	7.72	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}G	0.574	
	97182.555	97310	47.66	3d^3 4s 4p ^{4}P.^{3}P; ^{4}P	38.83	3d^3 4s 4p ^{4}P. ^{3}P; ^{6}S	1.756	
	97875.016	97864	60.60	3d^3 4s 4p ^{4}P.^{3}P; ^{6}S	31.99	3d^3 4s 4p ^{4}P. ^{3}P; ^{4}P	1.841	
	98207.461	98021	51.59	3d^4 4p ^{3}F; ^{2}D	18.56	3d^4 4p ^{3}F; ^{2}D	1.196	
	98641.891	98756	57.67	3d^3 4s 4p ^{2}G.^{3}P; ^{4}F	14.13	3d^4 4p ^{1}G; ^{2}F	0.985	
	99243.938	98911	35.46	3d^4 4p ^{1}G; ^{2}F	21.18	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}F	0.907	
		100798	52.35	3d^3 4s 4p ^{2}P.^{3}P; ^{4}P	27.08	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}P	1.586	
	101074.523	100857	45.68	3d^3 4s 4p ^{2}P.^{3}P; ^{4}D	29.69	3d^3 4s 4p ^{4}P. ^{3}P; ^{4}D	1.367	
	102145.641	102220	67.33	3d^3 4s 4p ^{2}G.^{3}P; ^{2}F	6.99	3d^4 4p ^{1}G; ^{2}F	0.877	
	102297.062	102442	41.13	3d^3 4s 4p ^{2}D.^{3}P; ^{4}F	12.77	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}F	1.042	
	102655.906	102815	43.71	3d^3 4s 4p ^{4}P.^{3}P; ^{4}D	40.54	3d^3 4s 4p ^{2}P. ^{3}P; ^{4}D	1.350	
	102678.945	102877	76.41	3d^3 4s 4p ^{4}F.^{1}P; ^{4}G	8.15	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}G	0.574	
		103278	45.91	3d^3 4s 4p ^{2}P.^{3}P; ^{2}D	24.43	3d^3 4s 4p ^{2}D. ^{3}P; ^{2}D	1.206	
	104467.805	104149	44.48	3d^3 4s 4p ^{2}D.^{3}P; ^{4}D	28.24	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}D	1.372	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	104869.117	104755	36.92	3d^3 4s 4p ^{4}F.^{1}P; ^{4}D	29.14	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}D	1.364	
	105121.969	105111	35.47	3d^4 4f^{5}D; ^{4}P	22.71	3d^4 4f^{5}D; ^{4}P	1.263	
		105139	38.74	3d^4 4f^{5}D; ^{6}H	34.64	3d^4 4f^{5}D; ^{4}P	0.976	
		105146	54.25	3d^4 4f^{5}D; ^{6}H	12.76	3d^4 4f^{5}D; ^{4}F	0.710	
		105289	39.12	3d^4 4f^{5}D; ^{6}D	33.09	3d^4 4f^{5}D; ^{6}P	1.641	
		105425	35.13	3d^4 4f^{5}D; ^{6}G	31.57	3d^4 4f^{5}D; ^{6}F	1.286	
		105470	38.03	3d^3 4s 4p ^{2}P.^{3}P; ^{4}P	35.43	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}P	1.587	
	105438.273	105561	46.61	3d^4 4f^{5}D; ^{6}G	17.89	3d^4 4f^{5}D; ^{6}D	1.256	
	105532.070	105631	60.64	3d^4 4f^{5}D; ^{4}D	11.14	3d^4 4f^{5}D; ^{6}P	1.410	
		105720	40.17	3d^4 4f^{5}D; ^{6}F	30.90	3d^4 4f^{5}D; ^{6}D	1.358	
	105677.609	105735	72.04	3d^4 4f^{5}D; ^{4}G	7.34	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}G	0.693	
	105902.969	106054	42.79	3d^4 4f^{5}D; ^{4}F	21.65	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}F	0.951	
		106170	60.26	3d^3 4s 4p ^{2}H.^{3}P; ^{4}G	9.79	3d^4 4f^{5}D; ^{4}G	0.656	
	107022.148	106930	46.88	3d^3 4s 4p ^{2}D.^{3}P; ^{2}F	27.17	3d^3 4s 4p ^{4}P. ^{3}P; ^{2}D	0.959	
	107355.516	107244	63.20	3d^3 4s 4p ^{4}P.^{3}P; ^{2}D	18.80	3d^3 4s 4p ^{2}D. ^{3}P; ^{2}F	1.098	
	109694.297	109633	96.24	3d^4 6p^{5}D; ^{6}F	1.51	3d^4 6p^{5}D; ^{4}F	1.314	
	109864.891	109769	42.29	3d^4 6p^{5}D; ^{6}P	34.27	3d^4 6p^{5}D; ^{4}P	1.730	
		109997	61.99	3d^4 6p^{5}D; ^{6}D	34.84	3d^4 6p^{5}D; ^{6}P	1.726	
	109943.383	110057	43.71	3d^3 4s 4p ^{2}D.^{3}P; ^{2}D	39.50	3d^3 4s 4p ^{2}P. ^{3}P; ^{2}D	1.202	
	109973.973	110194	53.11	3d^4 6p^{5}D; ^{4}P	21.81	3d^4 6p^{5}D; ^{6}P	1.656	
		110350	76.94	3d^4 5p ^{3}H; ^{4}G	11.07	3d^4 6p^{5}D; ^{4}F	0.640	
	110315.062	110396	75.77	3d^4 6p^{5}D; ^{4}F	12.02	3d^4 5p ^{3}H; ^{4}G	1.000	
		110823	47.79	3d^4 5p ^{3}P; ^{4}D	32.61	3d^4 5p ^{3}P; ^{4}D	1.379	
	111082.312	111171	83.53	3d^4 6p^{5}D; ^{4}D	5.12	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}D	1.371	
		111394	70.79	3d^4 5p ^{3}F; ^{4}G	21.54	3d^4 5p ^{3}F; ^{4}G	0.590	
		111430	45.94	3d^4 5p ^{3}P; ^{4}P	30.14	3d^4 5p ^{3}P; ^{4}P	1.536	
		111835	33.34	3d^4 5p ^{3}F; ^{4}F	18.85	3d^4 5p ^{3}F; ^{2}D	1.122	
		112122	37.80	3d^4 5p ^{3}P; ^{2}D	25.68	3d^4 5p ^{3}P; ^{2}D	1.203	
		112140	28.44	3d^4 5p ^{3}F; ^{4}F	13.29	3d^4 5p ^{3}F; ^{2}F	1.085	
		112264	37.84	3d^4 5p ^{3}F; ^{2}F	27.21	3d^4 5p ^{3}F; ^{4}D	1.071	
		112298	46.41	3d^4 5p ^{3}F; ^{2}D	14.09	3d^4 5p ^{3}F; ^{2}D	1.197	
		113107	60.39	3d^4 4p ^{1}D; ^{2}F	17.19	3d^4 4p ^{1}D; ^{2}F	0.861	
		113985	43.43	3d^4 5p ^{3}G; ^{4}G	24.93	3d^4 5p ^{3}G; ^{4}F	0.796	
		114198	39.32	3d^4 5p ^{3}G; ^{4}G	27.41	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}F	0.839	
		114515	68.91	3d^4 5p ^{3}G; ^{2}F	11.20	3d^4 5p ^{3}G; ^{4}G	0.837	
		115082	52.38	3d^4 5f^{5}D; ^{4}P	10.98	3d^4 5f^{5}D; ^{4}D	1.447	
		115117	38.60	3d^3 4s 4p ^{2}F.^{3}P; ^{4}F	28.81	3d^4 5p ^{3}G; ^{4}F	1.149	
	115208.312	115234	90.58	3d^4 5f^{5}D; ^{6}H	6.47	3d^4 5f^{5}D; ^{6}G	0.344	
	115309.562	115340	38.23	3d^4 5f^{5}D; ^{6}D	30.48	3d^4 5f^{5}D; ^{6}F	1.448	
		115426	24.94	3d^4 5f^{5}D; ^{4}D	23.38	3d^4 4p^{5}D; ^{6}G	1.231	
	115461.742	115486	26.03	3d^4 5f^{5}D; ^{4}G	23.51	3d^4 4p^{5}D; ^{6}G	1.068	
		115580	28.63	3d^4 5f^{5}D; ^{4}G	24.43	3d^4 4p^{5}D; ^{6}G	1.017	
	115767.047	115618	27.97	3d^4 5f^{5}D; ^{4}G	26.78	3d^4 4p^{5}D; ^{6}P	1.237	
		115722	69.55	3d^4 4p ^{1}D; ^{2}D	23.99	3d^4 4p ^{1}D; ^{2}D	1.199	
		115765	44.58	3d^4 5f^{5}D; ^{6}D	28.61	3d^4 5f^{5}D; ^{6}P	1.614	
	115810.297	115817	55.26	3d^4 5f^{5}D; ^{4}F	16.85	3d^4 5f^{5}D; ^{4}D	1.045	
		116243	64.53	3d^3 4s 4p ^{4}P.^{1}P; ^{4}P	21.19	3d^4 5f^{5}D; ^{4}P	1.597	
		116672	93.95	3d^3 4s 4p ^{2}F.^{3}P; ^{4}G	3.76	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}G	0.574	
		117131	55.24	3d^3 4s 4p ^{2}F.^{3}P; ^{4}D	29.93	3d^3 4s 4p ^{4}P. ^{1}P; ^{4}D	1.372	
		118054	36.66	3d^4 5p ^{1}G; ^{2}F	26.39	3d^3 4s 4p ^{2}G. ^{1}P; ^{2}F	0.858	
		118788	50.83	3d^3 4s 4p ^{4}P.^{1}P; ^{4}D	36.95	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}D	1.370	
		119248	30.82	3d^3 4s 4p ^{2}G.^{1}P; ^{2}F	26.33	3d^4 5p ^{3}D; ^{2}F	0.859	
		120046	51.79	3d^3 4s 4p ^{2}F.^{3}P; ^{2}D	16.03	3d^4 5p ^{3}D; ^{2}D	1.202	
		120365	76.53	3d^4 5p ^{3}D; ^{4}F	16.42	3d^4 5p ^{3}D; ^{4}D	1.093	
		120433	34.72	3d^4 5p ^{3}D; ^{2}D	23.53	3d^3 4s 4p ^{2}F. ^{3}P; ^{2}D	1.261	
		120726	48.34	3d^4 5p ^{3}D; ^{4}D	17.51	3d^4 5p ^{3}D; ^{4}F	1.273	
		120849	76.78	3d^4 4f ^{3}H; ^{4}G	17.99	3d^4 4f ^{3}H; ^{2}F	0.643	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
		120896	54.24	3d⁴ 4f ³H; ²F	23.60	3d⁴ 4f ³H; ⁴F	0.899	
		120992	70.02	3d⁴ 5p ³D; ⁴P	6.87	3d⁴ 4f ³H; ⁴D	1.509	
3.5								
	47227.219	47165	99.53	3d⁴ 4p ⁵D; ⁶F	0.24	3d⁴ 5p ⁵D; ⁶F	1.398	
	48632.059	48559	99.56	3d⁴ 4p⁵D; ⁶P	0.13	3d⁴ 5p⁵D; ⁶P	1.715	
	49645.805	49639	99.30	3d⁴ 4p⁵D; ⁶D	0.31	3d⁴ 4p⁵D; ⁴F	1.587	
	51788.816	51980	95.34	3d⁴ 4p⁵D; ⁴F	1.80	3d⁴ 4p ³F; ⁴F	1.240	
	54784.449	54707	97.20	3d⁴ 4p⁵D; ⁴D	0.92	3d⁴ 4p ³D; ⁴D	1.429	
	63600.863	63642	82.23	3d⁴ 4p ³H; ⁴H	16.09	3d⁴ 4p ³G; ⁴H	0.669	
	64924.461	64801	44.80	3d⁴ 4p ³P; ⁴D	31.52	3d⁴ 4p ³P; ⁴D	1.428	
	65256.852	65298	31.00	3d⁴ 4p ³H; ²G	22.87	3d⁴ 4p ³F; ⁴G	0.934	
	65542.898	65498	27.66	3d⁴ 4p ³H; ²G	27.29	3d⁴ 4p ³F; ⁴G	0.939	
	67333.781	67323	75.03	3d⁴ 4p ³F; ⁴F	14.53	3d⁴ 4p ³F; ⁴F	1.228	
	67393.453	67378	69.21	3d⁴ 4p ³H; ⁴G	17.47	3d⁴ 4p ³F; ⁴G	0.996	
	67875.367	68035	50.77	3d⁴ 4p ³F; ⁴D	14.36	3d⁴ 4p ³F; ⁴D	1.393	
	68759.805	68714	33.51	3d⁴ 4p ³F; ²F	25.44	3d⁴ 4p ³G; ²F	1.165	
	68843.273	68938	82.37	3d⁴ 4p ³G; ⁴H	16.12	3d⁴ 4p ³H; ⁴H	0.669	
	69506.070	69621	76.20	3d⁴ 4p ³G; ⁴F	9.02	3d⁴ 4p ³D; ⁴F	1.210	
	69903.477	69778	36.09	3d⁴ 4p ³F; ²G	24.67	3d⁴ 4p ³H; ²G	0.911	
	70426.992	70316	69.91	3d⁴ 4p ³G; ⁴G	12.89	3d⁴ 4p ³H; ⁴G	0.999	
	70852.164	70695	52.42	3d⁴ 4p ³G; ²F	33.12	3d⁴ 4p ³F; ²F	1.142	
	72648.516	72752	78.63	3d⁴ 4p ³G; ²G	10.37	3d⁴ 4p ³H; ²G	0.893	
	73485.609	73623	92.77	3d⁴ 4p ³D; ⁴D	2.62	3d⁴ 4p ³D; ⁴F	1.421	
	74114.367	74058	51.78	3d⁴ 4p ¹G; ²F	24.62	3d⁴ 4p ¹G; ²F	1.145	
	74423.672	74432	83.74	3d⁴ 4p ³D; ⁴F	10.17	3d⁴ 4p ³G; ⁴F	1.242	
	75716.495	75929	47.58	3d⁴ 4p ¹G; ²G	28.11	3d⁴ 4p ¹G; ²G	0.891	
	76878.953	76839	74.11	3d⁴ 4p ³D; ²F	7.47	3d⁴ 4p ³G; ²F	1.143	
		79328	99.85	3d³ 4s 4p ⁴F.³P; ⁶G	0.03	3d³ 4s 4p ⁴F. ³P; ⁴F	1.143	
	81432.227	81376	69.36	3d⁴ 4p ¹D; ²F	18.39	3d⁴ 4p ¹D; ²F	1.143	
	81978.047	82032	76.16	3d³ 4s 4p ⁴F.³P; ⁶D	21.26	3d³ 4s 4p ⁴F. ³P; ⁶F	1.547	
	82142.711	82126	78.30	3d³ 4s 4p ⁴F.³P; ⁶F	20.54	3d³ 4s 4p ⁴F. ³P; ⁶D	1.438	
	84677.117	84456	87.25	3d⁴ 4p ¹F; ²F	3.21	3d⁴ 4p ³D; ²F	1.141	
	85573.125	85562	94.02	3d⁴ 4p ¹F; ²G	1.26	3d⁴ 4p ¹G; ²G	0.892	
	86078.820	85981	89.48	3d³ 4s 4p ⁴F.³P; ⁴D	4.67	3d³ 4s 4p ⁴P. ³P; ⁴D	1.430	
	86797.242	86901	93.55	3d³ 4s 4p ⁴F.³P; ⁴G	3.79	3d³ 4s 4p ²G. ³P; ⁴G	0.985	
	87916.672	88239	74.86	3d³ 4s 4p ⁴F.³P; ⁴F	18.84	3d⁴ 4p ³F; ⁴F	1.238	
	90218.406	90078	56.38	3d⁴ 4p ³F; ⁴F	19.63	3d³ 4s 4p ⁴F. ³P; ⁴F	1.255	
	90489.844	90388	32.67	3d⁴ 4p ³P; ⁴D	23.42	3d⁴ 4p ³F; ⁴D	1.406	
	90830.844	91122	43.29	3d⁴ 4p ³F; ²F	16.63	3d⁴ 4p ³F; ⁴G	1.108	
	91122.859	91306	55.09	3d⁴ 4p ³F; ⁴G	18.26	3d⁴ 4p ³F; ⁴G	1.024	
		91658	89.81	3d³ 4s 4p ⁴F.³P; ²G	4.61	3d⁴ 4p ³F; ²G	0.892	
	92653.172	92738	68.21	3d³ 4s 4p ⁴P.³P; ⁶P	31.12	3d⁴ 5p⁵D; ⁶P	1.715	
	93276.853	93312	97.94	3d⁴ 5p⁵D; ⁶F	0.85	3d⁴ 5p⁵D; ⁴F	1.397	
		93458	66.06	3d³ 4s 4p ⁴F.³P; ²F	8.33	3d⁴ 4p ³F; ²F	1.191	
	93531.695	93602	38.12	3d⁴ 4p ³F; ⁴D	16.18	3d⁴ 4p ³P; ⁴D	1.380	
	93801.523	93833	72.90	3d⁴ 5p⁵D; ⁶D	22.47	3d³ 4s 4p ⁴P. ³P; ⁶D	1.582	
	93966.430	94116	65.37	3d⁴ 5p⁵D; ⁶P	30.80	3d³ 4s 4p ⁴P. ³P; ⁶P	1.705	
	94218.672	94236	73.12	3d³ 4s 4p ⁴P.³P; ⁶D	21.19	3d⁴ 5p⁵D; ⁶D	1.574	
	94452.672	94356	71.43	3d⁴ 4p ³F; ²G	20.30	3d⁴ 4p ³F; ²G	0.889	
	94522.305	94518	87.33	3d⁴ 5p⁵D; ⁴F	4.85	3d⁴ 5p⁵D; ⁶D	1.271	
	95250.680	95137	84.67	3d⁴ 5p⁵D; ⁴D	4.36	3d³ 4s 4p ⁴F. ¹P; ⁴D	1.429	
		96229	83.29	3d³ 4s 4p ²G.³P; ⁴H	15.04	3d³ 4s 4p ²H. ³P; ⁴H	0.670	
	97187.102	97262	49.60	3d⁴ 4p ¹G; ²G	27.94	3d⁴ 4p ¹G; ²G	0.898	
	97728.227	97450	77.85	3d³ 4s 4p ²G.³P; ⁴G	6.77	3d³ 4s 4p ⁴F. ¹P; ⁴G	0.975	
	98719.328	98578	46.29	3d⁴ 4p ¹G; ²F	20.34	3d⁴ 4p ¹G; ²F	1.145	
	99069.273	98959	76.87	3d³ 4s 4p ²G.³P; ⁴F	8.89	3d³ 4s 4p ²D. ³P; ⁴F	1.231	
	101514.195	101244	44.52	3d³ 4s 4p ²P.³P; ⁴D	31.10	3d³ 4s 4p ⁴P. ³P; ⁴D	1.398	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	101170.469	101298	54.81	3d^3 4s 4p ^{2}H.^{3}P; ^{4}H	24.28	3d^3 4s 4p ^{2}G. ^{3}P; ^{2}G	0.764	
	101864.180	102024	32.46	3d^3 4s 4p ^{2}G.^{3}P; ^{2}F	28.50	3d^3 4s 4p ^{2}G. ^{3}P; ^{2}G	0.951	
	102121.992	102264	33.30	3d^3 4s 4p ^{2}G.^{3}P; ^{2}F	26.94	3d^3 4s 4p ^{2}G. ^{3}P; ^{2}G	1.045	
	102492.539	102519	37.84	3d^3 4s 4p ^{2}D.^{3}P; ^{4}F	11.96	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}F	1.233	
	102831.602	102909	42.89	3d^3 4s 4p ^{2}P.^{3}P; ^{4}D	41.14	3d^3 4s 4p ^{4}P. ^{3}P; ^{4}D	1.404	
		103097	74.74	3d^3 4s 4p ^{4}F.^{1}P; ^{4}G	7.91	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}G	0.986	
	104680.789	104455	58.26	3d^3 4s 4p ^{2}D.^{3}P; ^{4}D	15.94	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}D	1.427	
		105005	40.42	3d^3 4s 4p ^{4}F.^{1}P; ^{4}D	18.89	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}D	1.411	
	105173.406	105172	49.84	3d^4 4f^{5}D; ^{6}P	21.34	3d^4 4f^{5}D; ^{6}D	1.469	
	105197.312	105186	59.61	3d^4 4f^{5}D; ^{6}H	13.65	3d^4 4f^{5}D; ^{4}H	0.991	
	105206.719	105267	68.35	3d^4 4f^{5}D; ^{4}H	12.22	3d^4 4f^{5}D; ^{6}H	0.795	
	105282.625	105302	41.16	3d^4 4f^{5}D; ^{4}F	18.76	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}F	1.188	
		105402	41.15	3d^4 4f^{5}D; ^{6}F	19.66	3d^4 4f^{5}D; ^{6}P	1.419	
	105419.961	105573	50.15	3d^4 4f^{5}D; ^{6}G	29.98	3d^4 4f^{5}D; ^{6}D	1.330	
	105507.531	105627	71.19	3d^4 4f^{5}D; ^{4}D	7.85	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}F	1.431	
		105769	52.33	3d^4 4f^{5}D; ^{6}F	22.48	3d^3 4s 4p^{5}D; ^{6}D	1.388	
	105724.656	105821	72.65	3d^4 4f^{5}D; ^{4}G	11.42	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}G	1.002	
	105985.555	106114	60.85	3d^3 4s 4p ^{2}H.^{3}P; ^{4}G	11.82	3d^4 4f^{5}D; ^{4}F	1.052	
	106779.250	106269	31.23	3d^4 4f^{5}D; ^{4}F	27.67	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}F	1.166	
	107153.039	107281	65.84	3d^3 4s 4p ^{2}D.^{3}P; ^{2}F	20.30	3d^3 4s 4p ^{2}D. ^{3}P; ^{2}F	1.143	
	107918.547	107604	83.07	3d^3 4s 4p ^{2}H.^{3}P; ^{2}G	9.91	3d^3 4s 4p ^{2}F. ^{3}P; ^{2}G	0.893	
		109048	88.75	3d^4 5p ^{3}H; ^{4}H	8.13	3d^4 5p ^{3}H; ^{2}G	0.688	
		109745	80.70	3d^4 5p ^{3}H; ^{2}G	9.01	3d^4 5p ^{3}H; ^{4}H	0.875	
	109812.039	109796	94.66	3d^4 5p^{5}D; ^{6}F	2.62	3d^4 6p^{5}D; ^{4}F	1.395	
	110097.094	110034	89.90	3d^4 5p^{5}D; ^{6}P	7.77	3d^4 6p^{5}D; ^{6}D	1.700	
	110272.117	110134	83.10	3d^4 5p^{5}D; ^{6}D	7.02	3d^4 6p^{5}D; ^{6}P	1.568	
		110400	81.90	3d^4 5p ^{3}H; ^{4}G	4.37	3d^4 5p ^{3}H; ^{2}G	0.990	
	110471.281	110506	80.88	3d^4 5p^{5}D; ^{4}F	7.32	3d^4 6p^{5}D; ^{6}D	1.265	
	111269.164	111265	35.91	3d^4 5p ^{3}P; ^{4}D	24.20	3d^4 5p ^{3}P; ^{4}D	1.426	
		111323	70.12	3d^4 5p^{5}D; ^{4}D	8.89	3d^4 5p ^{3}F; ^{4}D	1.429	
		111490	66.61	3d^4 5p ^{3}F; ^{4}G	20.00	3d^4 5p ^{3}F; ^{4}G	0.991	
		111999	39.93	3d^4 5p ^{3}F; ^{4}F	10.72	3d^4 5p ^{3}F; ^{4}F	1.256	
		112107	29.55	3d^4 5p ^{3}F; ^{2}G	15.72	3d^4 5p ^{3}F; ^{2}F	1.073	
		112228	33.16	3d^4 5p ^{3}F; ^{2}G	23.71	3d^4 5p ^{3}F; ^{4}F	1.087	
		112404	36.64	3d^4 5p ^{3}F; ^{2}F	27.34	3d^4 5p ^{3}F; ^{4}D	1.269	
		113366	60.04	3d^4 4p ^{1}D; ^{2}F	17.00	3d^4 4p ^{1}D; ^{2}F	1.143	
		113643	93.24	3d^4 5p ^{3}G; ^{4}H	2.29	3d^4 5p ^{3}G; ^{2}G	0.680	
		114056	38.23	3d^4 5p ^{3}G; ^{4}F	29.72	3d^4 5p ^{3}G; ^{4}G	1.153	
		114275	59.02	3d^4 5p ^{3}G; ^{4}G	16.66	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}F	1.056	
		114542	74.80	3d^4 5p ^{3}G; ^{2}G	6.72	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}F	0.926	
		114765	70.27	3d^4 5p ^{3}G; ^{2}F	7.20	3d^4 4p ^{1}D; ^{2}F	1.125	
		115149	42.79	3d^3 4s 4p ^{2}F.^{3}P; ^{4}F	34.90	3d^4 5p ^{3}G; ^{4}F	1.233	
	115249.250	115255	37.15	3d^4 5f^{5}D; ^{6}P	27.08	3d^4 5f^{5}D; ^{6}D	1.415	
	115309.094	115287	48.60	3d^4 5f^{5}D; ^{6}H	14.72	3d^4 5f^{5}D; ^{4}H	1.018	
	115398.391	115342	69.96	3d^4 5f^{5}D; ^{4}H	15.21	3d^4 5f^{5}D; ^{6}H	0.757	
	115447.578	115419	30.10	3d^4 5f^{5}D; ^{4}D	24.36	3d^4 5f^{5}D; ^{6}F	1.336	
		115474	29.61	3d^4 5f^{5}D; ^{4}D	16.25	3d^4 5f^{5}D; ^{6}P	1.328	
	115591.148	115599	44.20	3d^4 5f^{5}D; ^{6}G	22.86	3d^4 5f^{5}D; ^{6}D	1.349	
	115627.719	115649	55.05	3d^4 5f^{5}D; ^{4}G	20.48	3d^4 5f^{5}D; ^{4}D	1.140	
	115797.203	115789	44.59	3d^4 5f^{5}D; ^{6}F	35.91	3d^4 5f^{5}D; ^{6}D	1.453	
	115882.164	115889	55.63	3d^4 5f^{5}D; ^{4}F	24.87	3d^4 5f^{5}D; ^{4}G	1.189	
		116735	93.40	3d^3 4s 4p ^{2}F.^{3}P; ^{4}G	3.71	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}G	0.987	
		117045	64.44	3d^3 4s 4p ^{2}F.^{3}P; ^{4}D	22.29	3d^3 4s 4p ^{4}P. ^{1}P; ^{4}D	1.428	
		117526	41.94	3d^3 4s 4p ^{2}G.^{1}P; ^{2}G	26.01	3d^4 5p ^{1}G; ^{2}G	0.896	
		117964	43.43	3d^4 5p ^{1}G; ^{2}F	24.57	3d^4 5p ^{1}G; ^{2}F	1.136	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	118753.672	118835	59.56	3d^3 4s 4p ^{4}P.^{1}P; ^{4}D	27.64	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}D	1.429	
		119280	32.73	3d^3 4s 4p ^{2}G.^{1}P; ^{2}F	28.87	3d^4 5p ^{3}D; ^{2}F	1.119	
		119677	29.50	3d^4 5p ^{1}G; ^{2}G	26.52	3d^3 4s 4p ^{2}G. ^{1}P; ^{2}G	0.916	
		120439	71.90	3d^4 5p ^{3}D; ^{4}F	20.42	3d^4 5p ^{3}D; ^{4}D	1.277	
		120733	66.55	3d^4 5p ^{3}D; ^{4}D	23.67	3d^4 5p ^{3}D; ^{4}F	1.381	
		120790	82.87	3d^4 4f ^{3}H; ^{4}H	6.21	3d^4 4f ^{3}H; ^{4}G	0.712	
		120817	62.64	3d^3 4s 4p ^{2}F.^{3}P; ^{2}G	8.60	3d^3 4s 4p ^{2}H. ^{3}P; ^{2}G	0.893	
		120869	34.65	3d^4 4f ^{3}H; ^{4}G	34.04	3d^4 4f ^{3}H; ^{2}G	0.974	
		120948	41.92	3d^4 4f ^{3}H; ^{4}G	24.76	3d^4 4f ^{3}H; ^{2}F	0.979	
4.5								
	47464.559	47374	99.55	3d^4 4p ^{5}D; ^{6}F	0.24	3d^4 5p ^{5}D; ^{6}F	1.435	
	49838.379	49822	98.82	3d^4 4p ^{5}D; ^{6}D	0.81	3d^4 4p^{5}D; ^{4}F	1.555	
	51942.664	52116	95.05	3d^4 4p ^{5}D; ^{4}F	1.75	3d^4 4p ^{3}F; ^{4}F	1.336	
	63706.250	63740	81.82	3d^4 4p ^{3}H; ^{4}H	15.69	3d^4 4p ^{3}G; ^{4}H	0.969	
	65217.507	65183	94.74	3d^4 4p ^{3}H; ^{4}I	1.27	3d^4 4p ^{3}H; ^{2}G	0.742	
	65383.906	65388	33.21	3d^4 4p ^{3}F; ^{4}G	19.11	3d^4 4p ^{3}H; ^{2}G	1.150	
	65680.016	65651	35.75	3d^4 4p ^{3}H; ^{2}G	18.21	3d^4 4p ^{3}F; ^{2}G	1.120	
	67353.266	67339	71.14	3d^4 4p ^{3}H; ^{4}G	19.32	3d^4 4p ^{3}F; ^{4}G	1.172	
	67448.539	67441	78.72	3d^4 4p ^{3}F; ^{4}F	15.03	3d^4 4p ^{3}F; ^{4}F	1.330	
	68476.875	68335	80.59	3d^4 4p ^{3}H; ^{2}H	10.27	3d^4 4p ^{1}G; ^{2}H	0.912	
	68992.344	69073	82.82	3d^4 4p ^{3}G; ^{4}H	15.22	3d^4 4p ^{3}H; ^{4}H	0.971	
	69498.211	69609	74.26	3d^4 4p ^{3}G; ^{4}F	8.44	3d^4 4p ^{3}D; ^{4}F	1.302	
	70107.625	69979	33.56	3d^4 4p ^{3}F; ^{2}G	24.20	3d^4 4p ^{3}H; ^{2}G	1.132	
	70394.148	70376	65.03	3d^4 4p ^{3}G; ^{4}G	12.07	3d^4 4p ^{3}H; ^{4}G	1.160	
	70679.094	70844	74.48	3d^4 4p ^{3}G; ^{2}H	9.71	3d^4 4p ^{1}I; ^{2}H	0.930	
	72716.719	72847	75.57	3d^4 4p ^{3}G; ^{2}G	11.84	3d^4 4p ^{3}H; ^{2}G	1.111	
	74455.805	74501	88.13	3d^4 4p ^{3}D; ^{4}F	10.55	3d^4 4p ^{3}G; ^{4}F	1.334	
	74504.102	74584	49.98	3d^4 4p ^{1}G; ^{2}H	27.86	3d^4 4p ^{1}G; ^{2}H	0.911	
	75809.984	75997	45.64	3d^4 4p ^{1}G; ^{2}G	27.99	3d^4 4p ^{1}G; ^{2}G	1.110	
	77270.219	77010	86.10	3d^4 4p ^{1}I; ^{2}H	11.31	3d^4 4p ^{3}G; ^{2}H	0.910	
		79600	99.89	3d^3 4s 4p ^{4}F.^{3}P; ^{6}G	0.03	3d^4 4f^{5}D; ^{6}G	1.273	
	82192.180	82292	73.58	3d^3 4s 4p ^{4}F.^{3}P; ^{6}D	24.01	3d^3 4s 4p ^{4}F. ^{3}P; ^{6}F	1.527	
	82361.977	82359	75.56	3d^3 4s 4p ^{4}F.^{3}P; ^{6}F	23.45	3d^3 4s 4p ^{4}F. ^{3}P; ^{6}D	1.464	
	85939.023	85898	95.51	3d^4 4p ^{1}F; ^{2}G	1.28	3d^4 4p ^{1}G; ^{2}G	1.112	
	87092.562	87198	93.45	3d^3 4s 4p ^{4}F.^{3}P; ^{4}G	3.78	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}G	1.172	
	88073.438	88467	69.41	3d^3 4s 4p ^{4}F.^{3}P; ^{4}F	23.75	3d^4 4p ^{3}F; ^{4}F	1.333	
	90588.555	90201	58.77	3d^4 4p ^{3}F; ^{4}F	26.55	3d^3 4s 4p ^{4}F. ^{3}P; ^{4}F	1.332	
	91189.477	91343	71.99	3d^4 4p ^{3}F; ^{4}G	23.61	3d^4 4p ^{3}F; ^{4}G	1.172	
	92144.164	92057	88.00	3d^3 4s 4p ^{4}F.^{3}P; ^{2}G	6.71	3d^4 4p ^{3}F; ^{2}G	1.113	
	93444.000	93531	98.15	3d^4 5p^{5}D; ^{6}F	0.90	3d^4 4p^{5}D; ^{4}F	1.435	
	93641.531	94032	78.33	3d^4 5p^{5}D; ^{6}D	13.45	3d^3 4s 4p ^{4}P. ^{3}P; ^{6}D	1.542	
	94177.102	94214	70.29	3d^4 4p ^{3}F; ^{2}G	19.79	3d^4 4p ^{3}F; ^{2}G	1.112	
	94656.219	94493	76.50	3d^3 4s 4p ^{4}P.^{3}P; ^{6}D	14.25	3d^4 5p^{5}D; ^{4}F	1.524	
	94749.234	94708	77.01	3d^4 5p^{5}D; ^{4}F	13.53	3d^4 5p^{5}D; ^{6}D	1.381	
		96421	81.79	3d^3 4s 4p ^{2}G.^{3}P; ^{4}H	15.27	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}H	0.974	
	97333.133	97120	36.34	3d^4 4p ^{1}G; ^{2}H	19.98	3d^4 4p ^{1}G; ^{2}G	0.985	
	97480.148	97438	30.50	3d^4 4p ^{1}G; ^{2}G	19.83	3d^4 4p ^{1}G; ^{2}H	1.047	
	97904.352	97613	75.47	3d^3 4s 4p ^{2}G.^{3}P; ^{4}G	6.12	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}G	1.156	
	98812.539	99023	83.83	3d^3 4s 4p ^{2}G.^{3}P; ^{4}F	7.59	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}F	1.331	
	101296.547	101415	51.39	3d^3 4s 4p ^{2}H.^{3}P; ^{4}H	27.84	3d^3 4s 4p ^{2}G. ^{3}P; ^{2}G	1.017	
	101696.148	101834	39.57	3d^3 4s 4p ^{2}G.^{3}P; ^{2}H	20.47	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}H	0.944	
	101938.070	102070	40.67	3d^3 4s 4p ^{2}G.^{3}P; ^{2}G	22.91	3d^3 4s 4p ^{2}G. ^{3}P; ^{2}H	1.006	
	102725.547	102756	55.51	3d^3 4s 4p ^{2}D.^{3}P; ^{4}F	14.70	3d^3 4s 4p ^{2}D. ^{3}P; ^{4}F	1.332	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	103199.812	103055	84.89	3d^3 4s 4p ^{2}H.^{3}P; ^{4}I	10.96	3d^3 4s 4p ^{2}G. ^{3}P; ^{2}H	0.755	
	105203.461	103361	74.19	3d^3 4s 4p ^{4}F.^{1}P; ^{4}G	8.85	3d^4 4f^{5}D; ^{4}G	1.171	
	105263.438	105237	74.73	3d^4 4f^{5}D; ^{6}H	14.41	3d^4 4f^{5}D; ^{4}H	1.083	
	105398.156	105361	46.10	3d^4 4f^{5}D; ^{6}D	22.39	3d^4 4f^{5}D; ^{6}F	1.432	
	105406.898	105385	78.57	3d^4 4f^{5}D; ^{4}H	9.54	3d^4 4f^{5}D; ^{6}H	1.029	
		105471	51.45	3d^4 4f^{5}D; ^{4}F	16.65	3d^3 4s 4p ^{4}F. ^{1}P; ^{4}F	1.330	
	105623.547	105590	44.45	3d^4 4f^{5}D; ^{6}G	34.15	3d^4 4f^{5}D; ^{6}D	1.379	
		105777	80.76	3d^3 4s 4p ^{2}H.^{3}P; ^{2}H	13.69	3d^4 4f ^{2}G. ^{3}P; ^{2}H	0.914	
	105789.961	105809	51.78	3d^4 4f^{5}D; ^{6}F	36.60	3d^4 4f^{5}D; ^{6}G	1.383	
	106045.469	105925	60.91	3d^4 4f^{5}D; ^{4}G	24.66	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}G	1.175	
	106165.352	106159	57.52	3d^3 4s 4p ^{2}H.^{3}P; ^{4}G	17.91	3d^4 4f^{5}D; ^{4}G	1.183	
	106791.977	106452	47.99	3d^3 4s 4p ^{4}F.^{1}P; ^{4}F	28.49	3d^4 4f^{5}D; ^{4}F	1.318	
	107739.234	107403	82.87	3d^3 4s 4p ^{2}H.^{3}P; ^{2}G	9.12	3d^3 4s 4p ^{2}F. ^{3}P; ^{2}G	1.111	
		109021	69.74	3d^4 5p ^{3}H; ^{4}I	25.45	3d^4 5p ^{3}H; ^{4}H	0.798	
		109227	68.61	3d^4 5p ^{3}H; ^{4}H	24.53	3d^4 5p ^{3}H; ^{4}I	0.915	
		109843	51.57	3d^4 5p ^{3}H; ^{2}G	27.54	3d^4 5p ^{3}H; ^{2}H	1.046	
		110007	92.77	3d^4 6p^{5}D; ^{6}F	3.67	3d^4 6p^{5}D; ^{4}F	1.433	
		110083	61.32	3d^4 5p ^{3}H; ^{2}H	30.38	3d^4 5p ^{3}H; ^{2}G	0.974	
		110278	78.11	3d^4 6p ^{5}D; ^{6}D	15.04	3d^4 6p^{5}D; ^{4}F	1.513	
		110451	78.93	3d^4 5p ^{3}H; ^{4}G	7.71	3d^4 5p ^{3}H; ^{2}G	1.162	
	110665.477	110676	74.28	3d^4 6p^{5}D; ^{4}F	18.78	3d^4 6p^{5}D; ^{6}D	1.376	
		111628	61.25	3d^4 5p ^{3}F; ^{4}G	18.06	3d^4 5p ^{3}F; ^{4}G	1.176	
		112055	33.75	3d^4 5p ^{3}F; ^{4}F	24.58	3d^4 5p ^{3}F; ^{2}G	1.222	
		112309	37.97	3d^4 5p ^{3}F; ^{2}G	34.08	3d^4 5p ^{3}F; ^{4}F	1.211	
		113807	92.60	3d^4 5p ^{3}G; ^{4}H	1.42	3d^4 5p ^{3}G; ^{4}G	0.977	
		114120	47.57	3d^4 5p ^{3}G; ^{4}F	27.81	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}F	1.297	
		114334	57.88	3d^4 5p ^{3}G; ^{4}G	16.71	3d^4 5p ^{3}G; ^{2}H	1.142	
		114540	75.05	3d^4 5p ^{3}G; ^{2}H	16.87	3d^4 5p ^{3}G; ^{4}G	0.970	
		114726	77.87	3d^4 5p ^{3}G; ^{2}G	10.62	3d^3 4s 4p ^{2}F. ^{3}P; ^{4}F	1.131	
		115191	44.38	3d^3 4s 4p ^{2}F.^{3}P; ^{4}F	36.02	3d^4 5p ^{3}G; ^{4}F	1.318	
	115288.750	115314	56.30	3d^4 5f^{5}D; ^{6}H	17.06	3d^4 5f^{5}D; ^{6}G	1.134	
	115393.398	115414	41.43	3d^4 5f^{5}D; ^{6}D	31.93	3d^4 5f^{5}D; ^{6}F	1.402	
	115430.406	115452	71.62	3d^4 5f^{5}D; ^{4}H	13.82	3d^4 5f^{5}D; ^{6}H	1.020	
	115592.359	115597	46.25	3d^4 5f^{5}D; ^{6}G	36.21	3d^4 5f^{5}D; ^{6}D	1.365	
	115672.797	115695	40.75	3d^4 5f^{5}D; ^{4}G	40.59	3d^4 5f^{5}D; ^{4}F	1.234	
	115824.430	115812	53.73	3d^4 5f^{5}D; ^{6}F	28.62	3d^4 5f^{5}D; ^{6}G	1.402	
	115927.320	115933	47.46	3d^4 5f^{5}D; ^{4}F	43.38	3d^4 5f^{5}D; ^{4}G	1.254	
		116500	50.93	3d^4 5p ^{1}I; ^{2}H	37.89	3d^3 4s 4p ^{2}G. ^{1}P; ^{2}H	0.910	
		116809	93.62	3d^3 4s 4p ^{2}F.^{3}P; ^{4}G	3.66	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}G	1.174	
		117636	39.66	3d^3 4s 4p ^{2}G.^{1}P; ^{2}G	29.94	3d^4 5p ^{1}G; ^{2}G	1.108	
		118207	57.30	3d^4 5p ^{1}G; ^{2}H	31.36	3d^4 5p ^{1}G; ^{2}H	0.913	
		119484	44.61	3d^3 4s 4p ^{2}G.^{1}P; ^{2}H	32.14	3d^4 5p ^{1}I; ^{2}H	0.921	
		119848	29.56	3d^3 4s 4p ^{2}G.^{1}P; ^{2}G	27.72	3d^4 5p ^{1}G; ^{2}G	1.092	
		120614	98.24	3d^4 5p ^{3}D; ^{4}F	0.35	3d^4 5p ^{3}G; ^{4}F	1.332	
		120642	67.19	3d^4 4f ^{3}H; ^{2}H	10.50	3d^3 4s 4p ^{2}H. ^{1}P; ^{2}H	0.923	
		120750	80.84	3d^4 4f ^{3}H; ^{4}I	15.19	3d^4 4f ^{3}H; ^{4}H	0.775	
		120865	69.06	3d^4 4f ^{3}H; ^{4}H	13.76	3d^4 4f ^{3}H; ^{4}I	0.961	
		120953	43.13	3d^4 4f ^{3}H; ^{4}G	21.79	3d^4 4f ^{3}H; ^{2}G	1.143	
5.5								
	47751.602	47627	99.62	3d^4 4p ^{5}D; ^{6}F	0.24	3d^4 5p^{5}D; ^{6}F	1.456	
	63848.699	63870	82.32	3d^4 4p ^{3}H; ^{4}H	14.99	3d^4 4p ^{3}G; ^{4}H	1.131	
	65419.516	65362	97.57	3d^4 4p ^{3}H; ^{4}I	1.72	3d^4 4p ^{3}H; ^{4}H	0.968	
	65709.445	65744	45.69	3d^4 4p ^{3}F; ^{4}G	18.79	3d^4 4p ^{3}F; ^{4}G	1.271	
	67369.070	67356	67.97	3d^4 4p ^{3}H; ^{4}G	22.85	3d^4 4p ^{3}F; ^{4}G	1.271	
	67506.086	67689	91.76	3d^4 4p ^{3}H; ^{2}I	6.03	3d^4 4p ^{1}I; ^{2}I	0.927	
	68737.773	68566	83.15	3d^4 4p ^{3}H; ^{2}H	8.79	3d^4 4p ^{1}G; ^{2}H	1.092	
	69170.352	69237	83.41	3d^4 4p ^{3}G; ^{4}H	14.46	3d^4 4p ^{3}H; ^{4}H	1.133	

Table 5 (continued)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	70398.805	70399	70.07	$3d^4\,4p\ ^3G;\ ^2H$	10.52	$3d^4\,4p\ ^1I;\ ^2H$	1.114	
	70879.727	71024	67.98	$3d^4\,4p\ ^3G;\ ^4G$	11.94	$3d^4\,4p\ ^3H;\ ^4G$	1.249	
	74421.727	74286	86.40	$3d^4\,4p\ ^1I;\ ^2I$	5.25	$3d^4\,4p\ ^3H;\ ^2I$	0.937	
	74707.391	74793	47.53	$3d^4\,4p\ ^1G;\ ^2H$	25.38	$3d^4\,4p\ ^1G;\ ^2H$	1.079	
	77078.859	76811	84.75	$3d^4\,4p\ ^1I;\ ^2H$	11.95	$3d^4\,4p\ ^3G;\ ^2H$	1.090	
		79929	99.90	$3d^3\,4s\,4p\ ^4F.^3P;\ ^6G$	0.03	$3d^4\,4f^5D;\ ^6G$	1.343	
	82612.570	82613	99.43	$3d^3\,4s\,4p\ ^4F.^3P;\ ^6F$	0.21	$3d^3\,4s\,4p\ ^4F.\ ^3P;\ ^4G$	1.455	
	87450.438	87560	93.29	$3d^3\,4s\,4p\ ^4F.^3P;\ ^4G$	3.74	$3d^3\,4s\,4p\ ^2G.\ ^3P;\ ^4G$	1.274	
	91291.969	91433	73.43	$3d^4\,4p\ ^3F;\ ^4G$	23.63	$3d^4\,4p\ ^3F;\ ^4G$	1.273	
	93643.380	93799	99.46	$3d^4\,5p^5D;\ ^6F$	0.24	$3d^4\,4p^5D;\ ^6F$	1.456	
		96676	81.34	$3d^3\,4s\,4p\ ^2G.^3P;\ ^4H$	15.55	$3d^3\,4s\,4p\ ^2H.\ ^3P;\ ^4H$	1.136	
	97493.523	97499	56.25	$3d^4\,4p\ ^1G;\ ^2H$	28.87	$3d^4\,4p\ ^1G;\ ^2H$	1.096	
	97899.367	97781	81.44	$3d^3\,4s\,4p\ ^2G.^3P;\ ^4G$	5.98	$3d^3\,4s\,4p\ ^4F.\ ^1P;\ ^4G$	1.264	
	101782.969	101718	83.17	$3d^3\,4s\,4p\ ^2H.^3P;\ ^4H$	15.33	$3d^3\,4s\,4p\ ^2G.\ ^3P;\ ^4H$	1.134	
	101932.234	102124	69.60	$3d^3\,4s\,4p\ ^2G.^3P;\ ^2H$	13.48	$3d^3\,4s\,4p\ ^2H.\ ^3P;\ ^2H$	1.084	
		103155	93.20	$3d^3\,4s\,4p\ ^2H.^3P;\ ^4I$	4.64	$3d^3\,4s\,4p\ ^2G.\ ^3P;\ ^2H$	0.974	
	103513.555	103668	73.77	$3d^3\,4s\,4p\ ^4F.^1P;\ ^4G$	10.12	$3d^4\,4f^5D;\ ^4G$	1.273	
	105367.844	105330	79.22	$3d^4\,4f^5D;\ ^6H$	10.64	$3d^4\,4f^5D;\ ^4H$	1.211	
	105559.523	105526	84.63	$3d^4\,4f^5D;\ ^4H$	12.22	$3d^4\,4f^5D;\ ^6H$	1.146	
	105639.180	105595	58.42	$3d^4\,4f^5D;\ ^6F$	32.94	$3d^4\,4f^5D;\ ^6G$	1.396	
		105762	75.29	$3d^3\,4s\,4p\ ^2H.^3P;\ ^2H$	14.19	$3d^3\,4s\,4p\ ^2G.\ ^3P;\ ^2H$	1.104	
		105834	57.74	$3d^4\,4f^5D;\ ^6G$	39.32	$3d^4\,4f^5D;\ ^6F$	1.383	
	106032.141	106015	48.97	$3d^4\,4f^5D;\ ^4G$	38.24	$3d^3\,4s\,4p\ ^2H.\ ^3P;\ ^4G$	1.262	
		106271	44.46	$3d^3\,4s\,4p\ ^2H.^3P;\ ^4G$	36.02	$3d^4\,4f^5D;\ ^4G$	1.270	
	107850.148	107629	98.85	$3d^3\,4s\,4p\ ^2H.^3P;\ ^2I$	0.43	$3d^3\,4s\,4p\ ^2H.\ ^3P;\ ^2H$	0.924	
		109142	55.22	$3d^4\,5p\ ^3H;\ ^4I$	39.76	$3d^4\,5p\ ^3H;\ ^4H$	1.035	
		109402	56.81	$3d^4\,5p\ ^3H;\ ^4H$	40.97	$3d^4\,5p\ ^3H;\ ^4I$	1.064	
		109909	89.48	$3d^4\,5p\ ^3H;\ ^2I$	5.39	$3d^4\,5p\ ^3H;\ ^2H$	0.939	
		110070	67.82	$3d^4\,5p\ ^3H;\ ^2H$	17.91	$3d^4\,5p\ ^3H;\ ^4G$	1.116	
		110279	99.79	$3d^4\,6p\ ^5D;\ ^6F$	0.10	$3d^4\,5p^5D;\ ^6F$	1.456	
		110500	68.83	$3d^4\,5p\ ^3H;\ ^4G$	20.96	$3d^4\,5p\ ^3H;\ ^2H$	1.232	
		111889	75.21	$3d^4\,5p\ ^3F;\ ^4G$	21.82	$3d^4\,5p\ ^3F;\ ^4G$	1.271	
		113992	90.82	$3d^4\,5p\ ^3G;\ ^4H$	3.71	$3d^4\,5p\ ^3G;\ ^2H$	1.137	
		114387	65.95	$3d^4\,5p\ ^3G;\ ^4G$	24.49	$3d^4\,5p\ ^3G;\ ^2H$	1.218	
		114713	68.47	$3d^4\,5p\ ^3G;\ ^2H$	27.18	$3d^4\,5p\ ^3G;\ ^4G$	1.144	
	115396.773	115409	65.73	$3d^4\,5f^5D;\ ^6H$	17.89	$3d^4\,4f^5D;\ ^6G$	1.231	
	115585.117	115590	28.82	$3d^4\,5f^5D;\ ^6H$	26.38	$3d^3\,4s\,4p^5D;\ ^4H$	1.269	
	115598.883	115604	54.03	$3d^4\,5f^5D;\ ^4H$	26.72	$3d^4\,4p^5D;\ ^6F$	1.259	
	115840.391	115826	53.66	$3d^4\,5f^5D;\ ^6G$	41.58	$3d^4\,4p^5D;\ ^6F$	1.383	
	115916.148	115925	87.43	$3d^4\,5f^5D;\ ^4G$	7.93	$3d^3\,4s\,4p^5D;\ ^4H$	1.266	
		116516	59.53	$3d^4\,5p\ ^1I;\ ^2H$	29.10	$3d^3\,4s\,4p\ ^2G.\ ^1P;\ ^2H$	1.087	
		116889	94.76	$3d^3\,4s\,4p\ ^2F.^3P;\ ^4G$	3.63	$3d^3\,4s\,4p\ ^2H.\ ^3P;\ ^4G$	1.273	
		117240	93.51	$3d^4\,5p\ ^1I;\ ^2I$	2.43	$3d^3\,4s\,4p\ ^2H.\ ^1P;\ ^2I$	0.928	
		118451	56.37	$3d^4\,5p\ ^1G;\ ^2H$	30.71	$3d^4\,5p\ ^1G;\ ^2H$	1.091	
		119621	49.41	$3d^3\,4s\,4p\ ^2G.^1P;\ ^2H$	26.97	$3d^4\,5p\ ^1I;\ ^2H$	1.089	
		120664	56.15	$3d^4\,4f\ ^3H;\ ^2I$	23.09	$3d^4\,4f\ ^3H;\ ^2H$	0.968	
		120727	79.31	$3d^4\,4f\ ^3H;\ ^4K$	15.79	$3d^4\,4f\ ^3H;\ ^4I$	0.813	
		120793	39.81	$3d^4\,4f\ ^3H;\ ^4I$	36.30	$3d^4\,4f\ ^3H;\ ^2H$	1.011	
		120857	28.30	$3d^4\,4f\ ^3H;\ ^2I$	23.95	$3d^4\,4f\ ^3H;\ ^4I$	1.006	
		120951	60.81	$3d^4\,4f\ ^3H;\ ^4H$	17.40	$3d^4\,4f\ ^3H;\ ^4I$	1.103	
6.5								
	64030.504	64035	84.09	$3d^4\,4p\ ^3H;\ ^4H$	13.90	$3d^4\,4p\ ^3G;\ ^4H$	1.229	
	65617.945	65546	98.19	$3d^4\,4p\ ^3H;\ ^4I$	1.47	$3d^4\,4p\ ^3H;\ ^4H$	1.110	
	67588.875	67773	92.21	$3d^4\,4p\ ^3H;\ ^2I$	5.69	$3d^4\,4p\ ^1I;\ ^2I$	1.079	
	69388.148	69436	84.00	$3d^4\,4p\ ^3G;\ ^4H$	13.97	$3d^4\,4p\ ^3H;\ ^4H$	1.229	

Table 5 (*continued*)

J-value	E_{obs} (cm^{-1}) [8,27]	E_{calc} (cm^{-1})	Largest eigenvalue component (%)		Next largest eigenvalue component (%)		Calc. g_J	Obs. g_J [5]
	74424.156	74291	79.99	3d^4 4p ^{1}I; ^{2}K	19.28	3d^4 4p ^{1}I; ^{2}I	0.962	
	74743.180	74613	74.62	3d^4 4p ^{1}I; ^{2}I	19.73	3d^4 4p ^{1}I; ^{2}K	1.049	
		80313	99.89	3d^3 4s 4p ^{4}F.^{3}P; ^{6}G	0.06	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}H	1.385	
		97013	83.57	3d^3 4s 4p ^{2}G.^{3}P; ^{4}H	15.78	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}H	1.231	
	101900.578	101843	83.30	3d^3 4s 4p ^{2}H.^{3}P; ^{4}H	15.67	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}H	1.231	
		103317	99.50	3d^3 4s 4p ^{2}H.^{3}P; ^{4}I	0.20	3d^3 4s 4p ^{2}G. ^{3}P; ^{4}H	1.108	
		105455	87.40	3d^4 4f^{5}D; ^{6}H	6.50	3d^4 4f^{5}D; ^{6}G	1.286	
	105742.453	105691	91.40	3d^4 4f^{5}D; ^{4}H	7.65	3d^4 4f^{5}D; ^{6}H	1.236	
	105895.461	105832	92.58	3d^4 4f^{5}D; ^{6}G	4.91	3d^4 4f^{5}D; ^{6}H	1.377	
		107785	99.12	3d^3 4s 4p ^{2}H.^{3}P; ^{2}I	0.25	3d^4 5p ^{1}I; ^{2}I	1.077	
		109289	55.45	3d^4 5p ^{3}H; ^{4}H	37.27	3d^4 5p ^{3}H; ^{4}I	1.176	
		109554	61.14	3d^4 5p ^{3}H; ^{4}I	37.80	3d^4 5p ^{3}H; ^{4}H	1.155	
		110023	92.75	3d^4 5p ^{3}H; ^{2}I	5.24	3d^4 5p ^{3}H; ^{4}H	1.086	
		114228	98.81	3d^4 5p ^{3}G; ^{4}H	0.46	3d^4 5p ^{3}H; ^{4}H	1.231	
	115546.523	115543	80.16	3d^4 5f^{5}D; ^{6}H	13.05	3d^4 5f^{5}D; ^{6}G	1.293	
	115782.797	115774	82.52	3d^4 5f^{5}D; ^{4}H	12.47	3d^4 5f^{5}D; ^{6}H	1.245	
	115836.531	115822	81.99	3d^4 5f^{5}D; ^{6}G	10.60	3d^4 5f^{5}D; ^{4}H	1.362	
		117121	53.81	3d^4 5p ^{1}I; ^{2}I	44.33	3d^4 5p ^{1}I; ^{2}K	1.013	
		117468	55.38	3d^4 5p ^{1}I; ^{2}K	43.16	3d^4 5p ^{1}I; ^{2}I	0.997	
		120759	59.95	3d^4 4f ^{3}H; ^{4}K	21.11	3d^4 4f ^{3}H; ^{2}K	0.982	
		120811	60.58	3d^4 4f ^{3}H; ^{4}L	16.27	3d^4 4f ^{3}H; ^{2}I	0.890	
		120835	34.32	3d^4 4f ^{3}H; ^{2}I	31.32	3d^4 4f ^{3}H; ^{4}L	0.984	
		120895	51.96	3d^4 4f ^{3}H; ^{2}K	32.33	3d^4 4f ^{3}H; ^{4}I	0.997	
		120957	38.03	3d^4 4f ^{3}H; ^{2}I	27.49	3d^4 4f ^{3}H; ^{4}I	1.044	
7.5								
	65812.648	65731	99.72	3d^4 4p ^{3}H; ^{4}I	0.14	3d^4 5p ^{3}H; ^{4}I	1.200	
	74958.859	74838	99.80	3d^4 4p ^{1}I; ^{2}K	0.09	3d^4 5p ^{1}I; ^{2}K	1.067	
		103567	99.75	3d^3 4s 4p ^{2}H.^{3}P; ^{4}I	0.16	3d^4 5p ^{3}H; ^{4}I	1.200	
		105614	99.95	3d^4 4f^{5}D; ^{6}H	0.03	3d^4 4f ^{3}F; ^{4}I	1.334	
		109668	99.53	3d^4 5p ^{3}H; ^{4}I	0.16	3d^3 4s 4p ^{2}H. ^{3}P; ^{4}I	1.200	
	115734.766	115715	99.95	3d^4 5f^{5}D; ^{6}H	0.03	3d^4 5f ^{3}F; ^{4}I	1.334	
		117607	99.73	3d^4 5p ^{1}I; ^{2}K	0.11	3d^4 5p ^{3}H; ^{4}I	1.067	
		120819	36.33	3d^4 4f ^{3}H; ^{2}L	31.20	3d^4 4f ^{3}H; ^{4}L	0.998	
		120867	53.55	3d^4 4f ^{3}H; ^{4}K	18.92	3d^4 4f ^{3}H; ^{2}L	1.053	
		120941	51.51	3d^4 4f ^{3}H; ^{4}L	40.91	3d^4 4f ^{3}H; ^{2}L	0.964	
		120986	86.16	3d^4 4f ^{3}H; ^{4}I	11.87	3d^4 4f ^{3}H; ^{4}K	1.183	
8.5								
		120930	54.30	3d^4 4f ^{3}H; ^{4}L	27.93	3d^4 4f ^{3}H; ^{4}K	1.102	
		120982	71.89	3d^4 4f ^{3}H; ^{4}K	21.72	3d^4 4f ^{3}H; ^{4}L	1.148	
		121076	76.13	3d^4 4f ^{3}H; ^{2}L	23.73	3d^4 4f ^{3}H; ^{4}L	1.063	
9.5								
		121062	99.89	3d^4 4f ^{3}H; ^{4}L	0.11	3d^4 4f ^{1}I; ^{2}M	1.158	
		128722	99.89	3d^4 4f ^{1}I; ^{2}M	0.11	3d^4 4f ^{3}H; ^{4}L	1.053	
		131091	99.89	3d^4 5f ^{3}H; ^{4}L	0.11	3d^4 5f ^{1}I; ^{2}M	1.158	

Table 6
Values of the intra-configuration fine structure parameters for Cr II odd configurations.

Configuration	Parameter	Value (cm^{-1})
$3d^44p$	E_{av}	74271(10)
	$F^2(3d,3d)$	60474(54)
	$F^4(3d,3d)$	35556(83)
	$F^2(3d,4p)$	10838(88)
	$G^1(3d,4p)$	5081(38)
	$G^3(3d,4p)$	1023(74)
	ζ_{3d}	218(13)
	ζ_{4p}	254(19)
	α	54(1)
	β	−140(14)
	T_1	42(25)
	T_2	−237(38)
$3d^45p$	E_{av}	11874(30)
	$F^2(3d,3d)$	65945(530)
	$F^4(3d,3d)$	37859(518)
	$F^2(3d,5p)$	2619^d
	$G^1(3d,5p)$	1173^d
	$G^3(3d,5p)$	9406^d
	ζ_{3d}	218^d
	ζ_{5p}	81^d
	α	0^f
	β	0^f
	T_1	0^f
	T_2	0^f
$3d^46p$	E_{av}	134515(39)
	$F^2(3d,3d)$	64111(650)
	$F^4(3d,3d)$	38164(635)
	$F^2(3d,6p)$	1148^d
	$G^1(3d,6p)$	647^d
	$G^3(3d,6p)$	400^d
	ζ_{3d}	218^d
	ζ_{6p}	36^d
	α	0^f
	β	0^f
	T_1	0^f
	T_2	0^f
$3d^34s4p$	E_{av}	107441(14)
	$F^2(3d,3d)$	67824(127)
	$F^4(3d,3d)$	40200(146)
	$F^2(3d,4p)$	14457(177)
	$G^1(4s,4p)$	27810(105)
	$G^2(3d,4s)$	6507(191)
	$G^1(3d,4p)$	6166(110)
	$G^3(3d,4p)$	1576(287)
	ζ_{3d}	293(17)
	ζ_{4p}	382(57)
	α	53(1)
	β	−180(27)
	T_s	174(33)
	T_1	199(43)
	T_2	−207(41)
$3d^44f$	E_{av}	129606(27)
	$F^2(3d,3d)$	63513^d
	$F^4(3d,3d)$	37545^d
	$F^2(3d,4f)$	1000^d
	$F^4(3d,4f)$	200^d
	$G^1(3d,4f)$	130^d
	$G^3(3d,4f)$	77^d
	$G^5(3d,4f)$	0^f
	ζ_{3d}	220^d
	ζ_{4f}	0^f
	α	0^f
	β	0^f
	T_1	0^f
	T_2	0^f

Table 6 (*continued*)

Configuration	Parameter	Value (cm^{-1})
3d^{4}5f	E_{av}	139660(23)
	F^2(3d,3d)	63492^d
	F^4(3d,3d)	37554^d
	F^2(3d,5f)	510^d
	F^4(3d,5f)	120^d
	G^1(3d,5f)	100^d
	G^3(3d,5f)	55^d
	G^5(3d,5f)	0^f
	ζ_{3d}	220^d
	ζ_{5f}	0^f
	α	0^f
	β	0^f
	T$_1$	0^f
	T$_2$	0^f

^{f} Frozen to zero.
^{d} Deduced from *ab initio* or fs calculations.

Table 7
Values of odd configuration interaction parameters.

Configurations	Parameter[a]	Value (cm^{-1})
$3d^4 4p$–$3d^3 4s 4p$	R^2	$-5507(215)$
	D^2	$-4813(253)$
	E^1	-4813^d
$3d^4 4p$–$3d^4 5p$	E^1	$2389(224)$
	E^3	$1620(530)$
$3d^3 4s 4p$–$3d^4 5p$	D^2	$-3225(278)$
	E^1	$-3443(165)$

[a] For meaning of R^2, D^2, E^1 and E^3 see Cowan's book [28].
[d] Deduced from *ab initio* or fs calculations.