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Fundamental Configurations in Mo IV Spectrum

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Abstract

The spectrum of Mo IV was produced in a sliding-spark discharge and photographed with the 10.7 m normal-incidence vacuum spectrograph at the NBS in the 600–3200 Å spectral region. All 35 levels of the $4d^3$ and $4d^25s$ even configurations and all 45 of the levels of the $4d^25p$ odd configuration have been established from the 514 line classifications in the 800–3150 Å region. Parametric calculations have been made for the even level systems with configuration interaction and for the odd configuration.

1. Introduction

The fourth spectrum of molybdenum was analyzed originally by A. Y. Eliason [1] in 1933. He published 8 levels of the even configurations $4d^3$ and $4d^25s$ and 12 levels of the odd configuration $4d^25p$. We have studied these Mo IV fundamental configurations from new observations and established all of the 35 even and all of the 45 odd levels. We have confirmed Eliason's levels although the energy values have been slightly changed due to the better accuracy of the new observations.

2. Experimental method

The spectrum of molybdenum was photographed in the wavelength region 600–3200 Å using the NBS 10.7 m normal-incidence vacuum spectrograph equipped with a 12001/mm grating and having a plate factor of 0.77 Å/mm. A sliding-spark light source was used [2]. Discrimination of the ionization stages was made possible using peak current discharges between 30 and 500 A, producing a good separation of Mo III, Mo IV and Mo V lines. In some cases, it was necessary to introduce helium at approximately 20 Torr in order to maintain the discharge. The spectra were recorded on Kodak SWR plates in the wavelength region below 2500 Å and on 103a0 plates above 2500 Å. The intensity distribution along the spectral lines and the behaviour of the line intensity at different peak currents were used to attribute lines to the fourth spectrum.

The spectrograms were measured on the Abbe comparator at the Instituto de Optica in Madrid. The intensity of the lines are relative visual estimates of the photographic blackening. Almost all of the lines were measured at least three times. Reference lines of Cu I, Cu II, Ge I, Ge II, Ar I, Ar II [3] and impurity lines of O, C and Si [4] were used to calculate the wavelengths of the measured lines. Their uncertainty is estimated to be 0.005 Å.

The Mo V lines on our plates have been used in "A revision of the analysis of the fifth spectrum of Molybdenum

(Mo V)" [5]. The Mo III lines are being used in a revision and extension of the Mo^{++} ion spectrum now in progress.

3. Analysis

We first checked the 8 energy levels of $4d^3\ ^4F$ and $4d^2(^3F)5s\ ^4F$ from the even configurations and the 12 odd levels of the $4d^2(^3F)5p\ ^4G$, 4F and 4D terms, which were reported by Eliason [1]. All of his levels were confirmed, although the values have been slightly modified due to the better accuracy of our observations.

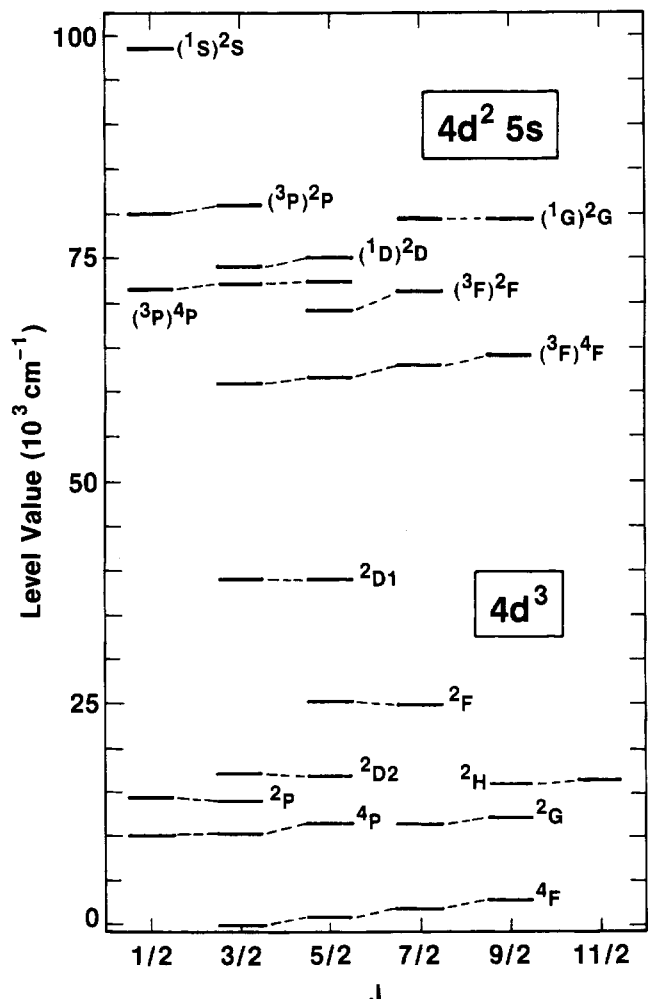


Fig. 1. Energy levels of the $4d^3$ and $4d^25s$ even configurations of triply ionized molybdenum. The levels are connected to form LS terms.

The wavenumber differences between these known levels were used with the observed lines to find new levels. The level structure, as predicted by parametric calculations, and the isoelectronic spectra, Zr II [6] and Nb III [7], were helpful in the search. Final energy level values were obtained using an iterative least-squares fitting of the levels to the observed classified lines.

A total of 508 lines were classified as belonging to the $4d^3-4d^25p$ and $4d^25s-4d^25p$ transition arrays of Mo IV. Six of these are doubly classified. Table I contains the wavelength, intensity, wavenumber and classification of each observed line, as well as the difference, $O-C$, between the observed and calculated wavelength. The $4d^3-4d^25p$ transition array falls in the 800–1400 Å region and that of the $4d^25s-4d^25p$ appears in the 1200–3130 Å region.

All of the 35 levels of the even configurations, $4d^3$ and $4d^25s$ are now known. A least squares fit of the radial coefficients to the observed energy levels, including configuration interaction, was made for these configurations.

We have found all 45 levels of the $4d^25p$ odd configuration. Levels of the $4d^25s5p$ configuration are not known but there is probably configuration interaction between levels of these two odd configurations. Therefore, the standard deviation of the least squares fit of the parameters to the levels of $4d^25p$ was larger than that for the even configurations.

Tables II and III give the relevant information about the even and odd levels, respectively. Included for each level in the tables are the configuration, term, J value, the level value and its uncertainty, and the number of observed transitions to or from the level. The tables also include the difference between the observed level value and that calculated with the least-squares fit parameters, $O-C$, and the leading eigenvector percentage(s) in LS coupling.

The levels of the even configurations, $4d^3$ and $4d^25s$, have an average purity of 90% in the LS coupling scheme. However, the $J = 3/2$ levels of $4d^3$ at 14 175 and 17 107 cm^{-1} are quite mixed as can be seen in Table II. Figure 1 is a graphical view of the level structure of the even configurations. The levels are connected to show the LS terms. The levels of the $4d^25p$ odd configuration have an average LS purity of 70%. Eight of these levels have leading LS percentage compositions of less than 50%. However only the level at 122 808 cm^{-1} , designated as $4d^2(1D)5p^2P_{3/2}$, is not named according to its largest eigenvector component. This leads to no ambiguity of the level names. Figure 2 shows the level structure of this configuration.

Table IV gives the parameters derived in the least-squares

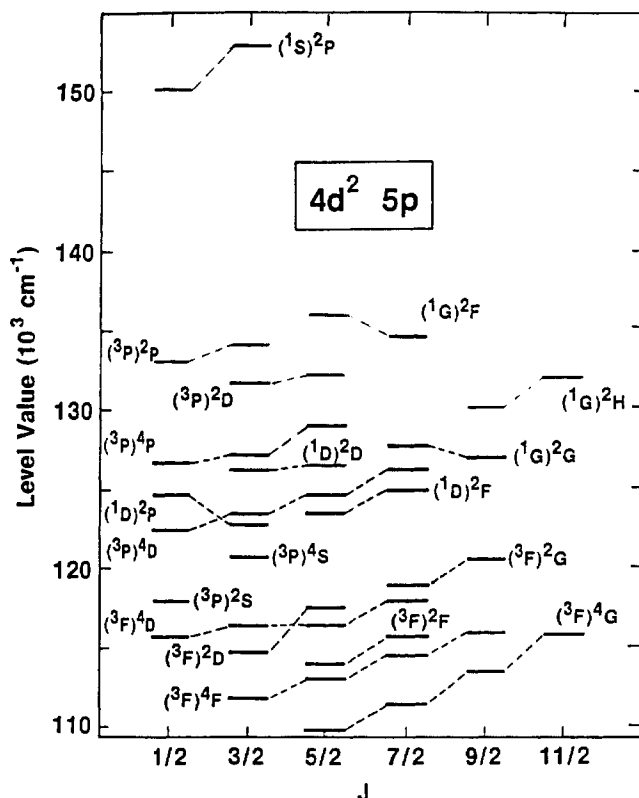


Fig. 2. Energy levels of the $4d^25p$ odd configuration of triply ionized molybdenum. The levels are connected to form LS terms.

fit mentioned above. The standard deviation for these even configurations was 30 cm^{-1} ; that for the $4d^25p$ was 141 cm^{-1} . The table also includes the relativistic Hartree–Fock values derived from the computer program of R. D. Cowan [8] as well as the ratio of the fitted to *ab initio* values.

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Table I. Classified lines of Mo IV

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification 4d ³ , 4d ² ()5s-4d ² ()5p
3137.700	2	31 861.24	-0.002	(³ P) ² P _{1/2} -(³ F) ⁴ F _{3/2} ⁰
3035.604	2	33 932.78	-0.001	(³ P) ² P _{3/2} -(³ F) ² F _{5/2} ⁰
2970.363	1	33 656.09	-0.005	(³ P) ² P _{3/2} -(³ F) ² D _{3/2} ⁰
2901.176	1	34 458.68	0.002	(¹ S) ² S _{1/2} -(³ P) ² P _{3/2} ⁰
2871.938	10	34 809.47	-0.003	(³ P) ² P _{1/2} -(³ F) ² D _{3/2} ⁰
2823.509	5	35 406.50	-0.002	(¹ D) ² D _{3/2} -(³ F) ⁴ G _{5/2} ⁰
2813.570	20	35 531.56	0.004	(³ P) ² P _{3/2} -(³ F) ⁴ D _{5/2} ⁰
2749.577	1	36 358.48	-0.002	(¹ D) ² D _{5/2} -(³ F) ⁴ G _{7/2} ⁰
2735.033	50	36 551.81	0.005	(³ P) ² P _{3/2} -(³ F) ² D _{3/2} ⁰
2727.272	100	36 655.82	0.006	(¹ G) ² G _{9/2} -(³ F) ² F _{7/2} ⁰
2724.939	10	36 687.20	0.000	(³ P) ² P _{1/2} -(³ F) ⁴ D _{3/2} ⁰
2712.486	5	36 855.62	0.002	(¹ G) ² G _{9/2} -(³ F) ⁴ F _{9/2} ⁰
2711.400	70	36 870.38	0.003	(³ P) ² P _{3/2} -(³ P) ² S _{1/2} ⁰
2648.126	1	37 751.31	-0.004	(¹ D) ² D _{3/2} -(³ F) ⁴ F _{3/2} ⁰
2634.665	2	37 944.17	-0.001	(¹ D) ² D _{5/2} -(³ F) ⁴ G _{5/2} ⁰
2629.140	50	38 023.91	-0.006	(³ P) ² P _{1/2} -(³ P) ² S _{1/2} ⁰
2568.836	10	38 916.47	-0.001	(¹ D) ² D _{3/2} -(³ F) ⁴ F _{5/2} ⁰
2563.067	1	39 004.06	-0.010	(¹ D) ² D _{5/2} -(³ F) ² F _{5/2} ⁰
2556.567	10	39 103.22	0.007	(³ P) ⁴ P _{5/2} -(³ F) ⁴ G _{7/2} ⁰
2511.251	20	39 808.80	-0.002	(¹ G) ² G _{7/2} -(³ F) ² G _{7/2} ⁰
2500.741	20	39 976.09	0.007	(¹ D) ² D _{3/2} -(³ F) ² F _{5/2} ⁰
2484.509	100	40 237.25	-0.004	(³ F) ² F _{5/2} -(³ F) ⁴ G _{5/2} ⁰
2456.300	1	40 699.31	0.009	(¹ D) ² D _{3/2} -(³ F) ² D _{3/2} ⁰
2451.374	50	40 781.09	-0.001	(¹ D) ² D _{5/2} -(³ F) ² F _{7/2} ⁰
2406.659	200	41 538.74	0.001	(¹ G) ² G _{9/2} -(³ F) ² G _{9/2} ⁰
2405.019	20	41 567.06	-0.008	(³ F) ² F _{7/2} -(³ F) ⁴ F _{5/2} ⁰
2375.436	20	42 084.68	0.002	(³ F) ² F _{7/2} -(³ F) ⁴ G _{9/2} ⁰
2371.103	20	42 161.58	-0.007	(³ F) ² F _{5/2} -(³ F) ⁴ G _{7/2} ⁰
2353.752	20	42 472.36	-0.018	(³ P) ⁴ P _{5/2} -(³ F) ² D _{3/2} ⁰
2347.701	10	42 581.82	0.007	(³ F) ² F _{5/2} -(³ F) ⁴ F _{3/2} ⁰
2310.560	1	43 266.24	-0.003	(³ F) ² F _{7/2} -(³ F) ⁴ F _{7/2} ⁰
2285.161	100	43 747.09	0.004	(³ F) ² F _{5/2} -(³ F) ⁴ F _{5/2} ⁰
2276.496	1	43 913.59	0.013	(¹ D) ² D _{3/2} -(³ P) ² S _{1/2} ⁰
2270.015	1	44 038.95	0.003	(³ P) ⁴ P _{1/2} -(³ F) ⁴ D _{1/2} ⁰
2251.363	300	44 403.77	0.004	(³ F) ² F _{7/2} -(³ F) ² F _{7/2} ⁰
2250.495	2	44 420.90	0.005	(³ P) ⁴ P _{3/2} -(³ F) ⁴ D _{3/2} ⁰
2250.391	1	44 422.95	0.011	(³ P) ⁴ P _{3/2} -(³ F) ⁴ D _{3/2} ⁰
2241.281	5	44 603.49	0.005	(³ F) ² F _{7/2} -(³ F) ⁴ F _{9/2} ⁰
2231.106	500	44 806.89	0.001	(³ F) ² F _{5/2} -(³ F) ² F _{5/2} ⁰
2229.676	1	44 835.62	0.000	(³ P) ⁴ P _{1/2} -(³ F) ⁴ D _{3/2} ⁰
2210.463	50	45 225.29	0.011	(³ F) ² F _{7/2} -(³ F) ⁴ D _{3/2} ⁰
2203.525	20	45 367.67	0.010	(³ P) ⁴ P _{5/2} -(³ F) ² D _{3/2} ⁰
2199.958	2	45 441.22	0.001	(³ P) ⁴ P _{3/2} -(³ F) ² D _{3/2} ⁰
2195.678	100	45 529.79	0.018	(³ F) ² F _{5/2} -(³ F) ² D _{3/2} ⁰
2187.110	1	45 708.13	0.006	(³ P) ² P _{3/2} -(³ P) ⁴ P _{1/2} ⁰
2184.917	20	45 754.01	-0.002	(¹ G) ² G _{7/2} -(¹ D) ² F _{7/2} ⁰
2180.634	100	45 843.86	0.005	(³ P) ⁴ P _{5/2} -(³ F) ⁴ D _{7/2} ⁰
2167.144	200	46 129.20	-0.010	(³ P) ² P _{3/2} -(³ P) ⁴ P _{3/2} ⁰
2161.680	200	46 245.79	-0.001	(³ F) ² F _{7/2} -(³ F) ² D _{3/2} ⁰
2157.099	20	46 343.99	0.019	(³ P) ² P _{1/2} -(¹ D) ² D _{3/2} ⁰
2145.976	2	46 584.17	-0.004	(³ F) ² F _{5/2} -(³ F) ² F _{5/2} ⁰
2139.651	100	46 721.86	0.000	(³ F) ² F _{7/2} -(³ F) ⁴ D _{7/2} ⁰
2137.614	1	46 766.38	-0.012	(³ P) ⁴ P _{5/2} -(³ F) ² G _{7/2} ⁰
2135.399	1	46 814.88	-0.009	(¹ D) ² D _{3/2} -(³ P) ⁴ S _{5/2} ⁰
2116.955	100	47 222.71	0.002	(¹ G) ² G _{7/2} -(³ P) ⁴ D _{7/2} ⁰
2113.040	5	47 310.19	-0.006	(¹ G) ² G _{9/2} -(³ P) ⁴ D _{7/2} ⁰
2108.775	20	47 405.87	-0.006	(³ F) ² F _{5/2} -(³ F) ⁴ F _{5/2} ⁰
2098.250	200	47 643.63	0.017	(³ F) ² F _{7/2} -(³ F) ² G _{7/2} ⁰
2091.864	400	47 789.06	0.000	(³ F) ⁴ F _{5/2} -(³ F) ⁴ G _{5/2} ⁰
2091.142	200	47 805.56	-0.001	(¹ G) ² G _{7/2} -(¹ G) ² G _{9/2} ⁰
2090.169	300	47 827.81	-0.002	(¹ D) ² D _{5/2} -(¹ D) ² P _{3/2} ⁰
2089.390	2	47 845.64	-0.003	(³ P) ² P _{3/2} -(³ P) ⁴ P _{5/2} ⁰
2087.328	500	47 892.90	-0.003	(¹ G) ² G _{9/2} -(¹ G) ² G _{9/2} ⁰
2065.010	20	48 410.44	0.002	(¹ D) ² D _{3/2} -(³ P) ⁴ D _{1/2} ⁰
2064.345	10	48 426.03	-0.001	(³ F) ² F _{5/2} -(³ F) ² D _{3/2} ⁰
2063.249	300	48 451.75	0.000	(¹ D) ² D _{5/2} -(³ P) ⁴ D _{3/2} ⁰

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification 4d ³ , 4d ² ()5s-4d ² ()5p
2060.398	500	48 518.79	0.007	(³ F) ⁴ F _{3/2} -(³ F) ⁴ G _{5/2} ⁰
2059.704	300	48 535.14	0.005	(¹ G) ² G _{7/2} -(¹ G) ² G _{7/2} ⁰
2058.946	100	48 553.00	0.005	(¹ D) ² D _{3/2} -(¹ D) ² F _{5/2} ⁰
2057.495	400	48 587.24	0.001	(³ P) ⁴ P _{3/2} -(³ P) ⁴ S _{3/2} ⁰
2055.999	2	48 622.59	-0.001	(¹ G) ² G _{9/2} -(¹ G) ² G _{7/2} ⁰
2055.641	500	48 631.05	-0.001	(³ F) ⁴ F _{7/2} -(³ F) ⁴ G _{7/2} ⁰
2054.391	200	48 660.64	0.000	(³ P) ⁴ P _{3/2} -(³ P) ⁴ S _{3/2} ⁰
2048.504	2	48 800.46	-0.017	(¹ D) ² D _{3/2} -(¹ D) ² P _{3/2} ⁰
2044.252	100	48 901.95	0.006	(³ F) ² F _{5/2} -(³ F) ⁴ D _{5/2} ⁰
2037.130	100	49 072.89	0.008	(³ P) ⁴ P _{1/2} -(³ P) ⁴ S _{3/2} ⁰
2028.300	600	49 286.50	0.009	(³ F) ² F _{7/2} -(³ F) ² G _{9/2} ⁰
2023.779	600	49 396.59	-0.001	(³ F) ⁴ F _{7/2} -(³ F) ⁴ G _{9/2} ⁰
2022.657	5	49 423.98	0.003	(¹ D) ² D _{3/2} -(³ P) ⁴ D _{3/2} ⁰
2018.515	400	49 525.39	0.001	(¹ D) ² D _{3/2} -(¹ D) ² F _{5/2} ⁰
2011.252	2	49 704.21	0.001	(¹ G) ² G _{7/2} -(³ P) ⁴ P _{5/2} ⁰
2010.889	700	49 713.18	0.006	(³ F) ⁴ F _{5/2} -(³ F) ⁴ G _{7/2} ⁰
2007.036	200	49 808.60	0.003	(¹ D) ² D _{5/2} -(³ P) ⁴ D _{3/2} ⁰
2006.411	500	49 824.11	0.006	(³ F) ² F _{5/2} -(³ F) ² G _{7/2} ⁰
2000.700	200	49 966.31	0.006	(¹ D) ² D _{5/2} -(³ F) ² F _{7/2} ⁰
1994.663	400	50 133.78	0.002	(³ F) ⁴ F _{5/2} -(³ F) ⁴ F _{3/2} ⁰
1991.374	400	50 216.58	0.006	(³ F) ⁴ F _{7/2} -(³ F) ⁴ F _{5/2} ⁰
1989.794	100	50 256.45	-0.001	(³ P) ⁴ P _{3/2} -(³ P) ⁴ D _{3/2} ⁰
1988.645	200	50 285.50	-0.003	(¹ S) ² S _{1/2} -(¹ S) ² P _{1/2} ⁰
1977.144	300	50 578.00	0.001	(³ F) ⁴ F _{9/2} -(³ F) ⁴ F _{7/2} ⁰
1974.494	300	50 645.88	0.005	(³ P) ⁴ P _{3/2} -(¹ D) ² P _{3/2} ⁰
1973.559	300	50 668.85	0.002	(³ P) ⁴ P _{1/2} -(³ P) ⁴ D _{1/2} ⁰
1971.114	200	50 732.73	0.005	(¹ D) ² D _{3/2} -(¹ D) ² P _{3/2} ⁰
1971.045	600	50 734.50	0.000	(³ F) ⁴ F _{7/2} -(³ F) ⁴ G _{9/2} ⁰
1969.242	300	50 780.96	0.001	(¹ D) ² D _{3/2} -(³ P) ⁴ D _{3/2} ⁰
1966.043	400	50 863.58	0.006	(³ F) ⁴ F _{3/2} -(³ F) ⁴ F _{3/2} ⁰
1962.487	300	50 955.75	0.001	(¹ G) ² G _{7/2} -(¹ G) ² H _{9/2} ⁰
1959.130	200	51 043.06	0.000	(¹ G) ² G _{9/2} -(¹ G) ² F _{9/2} ⁰
1954.394	300	51 166.75	0.004	(³ P) ² P _{3/2} -(³ P) ² D _{3/2} ⁰
1953.255	20	51 196.59	0.001	(³ P) ⁴ P _{5/2} -(³ P) ⁴ D _{3/2} ⁰
1950.760	200	51 262.07	0.002	(¹ D) ² D _{5/2} -(¹ D) ² D _{3/2} ⁰
1950.460	300	51 269.95	0.002	(³ P) ⁴ P _{3/2} -(³ P) ⁴ D _{3/2} ⁰
1950.214	50	51 276.42	0.002	(³ F) ⁴ F _{7/2} -(³ F) ² F _{9/2} ⁰
1949.360	500	51 298.88	0.006	(³ F) ⁴ F _{5/2} -(³ F) ⁴ F _{5/2} ⁰
1946.610	200	51 371.35	0.000	(³ P) ⁴ P _{3/2} -(¹ D) ² F _{5/2} ⁰
1944.197	300	51 435.11	0.005	(¹ D) ² D _{5/2} -(³ P) ⁴ D _{5/2} ⁰
1936.283	200	51 645.34	0.002	(³ F) ² F _{5/2} -(³ P) ⁴ S _{3/2} ⁰
1934.899	400	51 682.28	0.007	(³ P) ⁴ P _{1/2} -(³ P) ⁴ D _{3/2} ⁰
1933.653	400	51 715.58	0.004	(³ F) ⁴ F _{9/2} -(³ F) ² F _{7/2} ⁰
1932.906	300	51 735.57	0.000	(¹ D) ² D _{5/2} -(¹ D) ² D _{5/2} ⁰
1930.467	300	51 800.93	0.003	(³ P) ² P _{1/2} -(³ P) ² D _{3/2} ⁰
1929.210	900	51 834.68	-0.001	(³ F) ⁴ F _{9/2} -(³ F) ⁴ G _{11/2} ⁰
1926.200	800	51 915.68	-0.009	(³ F) ⁴ F

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification
				$4d^3, 4d^2()5s-4d^2()5p$
1884.883	300	53 053.69	-0.001	$(^3F)^4F_{7/2}-(^3F)^2F_{9/2}^0$
1883.875	200	53 082.07	-0.001	$(^3F)^4F_{5/2}-(^3F)^2D_{3/2}^0$
1883.642	500	53 088.64	0.002	$(^3F)^4F_{3/2}-(^3F)_{5/2}^0$
1880.685	300	53 172.11	0.011	$(^1D)^2D_{3/2}-(^3P)^4P_{3/2}^0$
1880.043	500	53 190.27	0.001	$(^3P)^2P_{3/2}-(^3P)^2P_{3/2}^0$
1877.814	700	53 253.41	0.000	$(^3F)^4F_{7/2}-(^3F)^4F_{9/2}^0$
1871.557	100	53 431.44	0.000	$(^3F)^2F_{7/2}-(^3P)^4D_{5/2}^0$
1870.446	300	53 463.18	0.000	$(^3P)^2P_{1/2}-(^3P)^2P_{1/2}^0$
1866.047	400	53 589.21	0.000	$(^3F)^2F_{7/2}-(^1D)^2F_{9/2}^0$
1864.605	300	53 630.66	0.004	$(^3F)^2F_{5/2}-(^1D)^2P_{3/2}^0$
1858.328	600	53 811.81	0.005	$(^3F)^4F_{3/2}-(^3F)^2D_{3/2}^0$
1856.137	500	53 875.33	-0.001	$(^3F)^4F_{3/2}-(^3F)^4D_{5/2}^0$
1851.613	100	54 006.96	0.001	$(^3P)^4P_{5/2}-(^1D)^2D_{3/2}^0$
1850.700	700	54 033.60	0.003	$(^3F)^4F_{9/2}-(^3F)^4D_{7/2}^0$
1849.091	200	54 080.62	-0.009	$(^3P)^4P_{3/2}-(^1D)^2D_{3/2}^0$
1847.198	400	54 136.04	-0.003	$(^3F)^4F_{5/2}-(^3F)^2F_{7/2}^0$
1845.690	700	54 180.27	-0.005	$(^3P)^4P_{5/2}-(^3P)^4D_{7/2}^0$
1843.140	20	54 255.23	-0.016	$(^3F)^2F_{5/2}-(^3P)^4D_{3/2}^0$
1840.136	10	54 343.80	-0.003	$(^3P)^2P_{1/2}-(^3P)^2P_{3/2}^0$
1839.714	300	54 356.27	-0.005	$(^3F)^2F_{5/2}-(^1D)^2F_{9/2}^0$
1835.521	400	54 460.44	0.000	$(^3P)^4P_{5/2}-(^1D)^2D_{3/2}^0$
1835.094	200	54 493.12	-0.010	$(^3P)^4P_{1/2}-(^1D)^2D_{3/2}^0$
1833.047	600	54 553.97	-0.005	$(^3P)^4P_{3/2}-(^1D)^2D_{3/2}^0$
1831.575	500	54 597.81	-0.006	$(^3P)^4P_{3/2}-(^3P)^4P_{1/2}^0$
1821.853	300	54 889.17	-0.005	$(^1D)^2D_{3/2}-(^3P)^4P_{3/2}^0$
1821.718	500	54 893.23	-0.005	$(^3F)^4F_{3/2}-(^3F)^4D_{1/2}^0$
1821.635	500	54 895.73	-0.005	$(^3F)^4F_{7/2}-(^3F)^2D_{3/2}^0$
1820.005	300	54 944.90	0.003	$(^3P)^4P_{5/2}-(^3P)^4P_{3/2}^0$
1819.575	500	54 957.88	-0.009	$(^3F)^4F_{5/2}-(^3F)^4D_{3/2}^0$
1819.500	600	54 960.15	-0.011	$(^3F)^4F_{5/2}-(^3F)^4D_{3/2}^0$
1817.842	200	55 010.28	-0.006	$(^3P)^4P_{1/2}-(^3P)^4P_{1/2}^0$
1817.572	200	55 018.45	-0.003	$(^3P)^4P_{3/2}-(^3P)^4P_{3/2}^0$
1816.251	5	55 058.46	-0.015	$(^3F)^2F_{7/2}-(^3P)^4D_{3/2}^0$
1809.219	50	55 272.46	-0.008	$(^3P)^2P_{3/2}-(^1G)^2F_{9/2}^0$
1806.405	200	55 358.57	-0.008	$(^3F)^2F_{7/2}-(^1D)^2D_{3/2}^0$
1805.964	500	55 372.08	-0.014	$(^3F)^4F_{7/2}-(^3F)^4D_{7/2}^0$
1804.047	500	55 430.92	-0.003	$(^3P)^4P_{1/2}-(^3P)^4P_{3/2}^0$
1797.233	500	55 641.08	-0.010	$(^3F)^2F_{7/2}-(^1G)^2G_{9/2}^0$
1795.726	50	55 687.78	-0.008	$(^3F)^4F_{3/2}-(^3F)^4D_{3/2}^0$
1795.651	200	55 690.10	-0.013	$(^3F)^4F_{3/2}-(^3F)^4D_{3/2}^0$
1793.476	300	55 757.64	-0.005	$(^1G)^2G_{7/2}-(^1G)^2F_{7/2}^0$
1793.089	300	55 769.68	-0.007	$(^3F)^2F_{5/2}-(^1D)^2F_{9/2}^0$
1790.672	700	55 844.95	-0.005	$(^1G)^2G_{9/2}-(^1G)^2F_{9/2}^0$
1786.418	300	55 977.94	-0.002	$(^3F)^4F_{5/2}-(^3F)^2D_{3/2}^0$
1776.385	300	56 294.10	-0.009	$(^3F)^4F_{7/2}-(^3F)^2G_{9/2}^0$
1773.974	200	56 370.61	-0.003	$(^3F)^2F_{7/2}-(^1G)^2G_{7/2}^0$
1766.826	300	56 598.66	-0.003	$(^3F)^4F_{9/2}-(^3F)^2G_{9/2}^0$
1764.866	200	56 661.52	0.002	$(^3P)^4P_{5/2}-(^3P)^4P_{3/2}^0$
1763.423	50	56 707.89	-0.003	$(^3F)^4F_{3/2}-(^3F)^2D_{3/2}^0$
1763.087	50	56 718.69	0.002	$(^1D)^2D_{5/2}-(^3P)^2D_{3/2}^0$
1762.581	300	56 734.98	-0.001	$(^3P)^4P_{3/2}-(^3P)^4P_{3/2}^0$
1753.562	20	57 026.78	-0.013	$(^3F)^4F_{3/2}-(^3P)^2S_{1/2}^0$
1752.375	200	57 065.41	-0.009	$(^3F)^2F_{5/2}-(^1D)^2D_{3/2}^0$
1750.368	500	57 130.84	0.001	$(^1G)^2G_{7/2}-(^1G)^2F_{5/2}^0$
1742.877	20	57 376.39	-0.008	$(^3F)^4F_{5/2}-(^3F)^2G_{9/2}^0$
1733.366	100	57 691.22	-0.005	$(^1D)^2D_{3/2}-(^3P)^2D_{3/2}^0$
1726.017	5	57 936.85	-0.010	$(^3F)^4F_{7/2}-(^3F)^2F_{9/2}^0$
1724.043	10	58 003.19	-0.002	$(^3F)^2F_{5/2}-(^3P)^4P_{3/2}^0$
1717.905	100	58 210.43	-0.004	$(^1D)^2D_{3/2}-(^3P)^2D_{3/2}^0$
1707.912	200	58 550.92	-0.005	$(^3F)^2F_{5/2}-(^1G)^2G_{7/2}^0$
1700.933	100	58 791.26	-0.007	$(^3F)^2F_{7/2}-(^1G)^2H_{9/2}^0$
1689.265	20	59 197.34	-0.002	$(^3F)^4F_{5/2}-(^3P)^4S_{3/2}^0$
1687.437	10	59 261.47	-0.001	$(^1D)^2D_{5/2}-(^3P)^2P_{3/2}^0$
1684.828	20	59 353.24	-0.001	$(^1D)^2D_{3/2}-(^3P)^2P_{1/2}^0$
1681.696	20	59 463.77	-0.004	$(^3P)^4P_{5/2}-(^3P)^2D_{3/2}^0$
1679.625	100	59 537.09	-0.003	$(^3P)^4P_{3/2}-(^3P)^2D_{3/2}^0$

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification
				$4d^3, 4d^2()5s-4d^2()5p$
1674.491	5	59 719.64	0.002	$(^3F)^2F_{5/2}-(^3P)^4P_{5/2}^0$
1668.072	10	59 949.45	0.000	$(^3P)^4P_{1/2}-(^3P)^2D_{3/2}^0$
1660.198	20	60 233.77	-0.001	$(^1D)^2D_{2/3}-(^3P)^2P_{3/2}^0$
1644.038	200	60 825.84	-0.004	$(^3F)^4F_{7/2}-(^1D)^2F_{9/2}^0$
1643.090	300	60 860.93	-0.005	$(^3F)^2F_{7/2}-(^3P)^2D_{3/2}^0$
1642.005	200	60 901.15	-0.002	$(^3F)^4F_{9/2}-(^1D)^2F_{9/2}^0$
1634.460	200	61 182.28	0.010	$(^3F)^4F_{5/2}-(^1D)^2P_{3/2}^0$
1634.008	10	61 199.21	-0.001	$(^3P)^4P_{3/2}-(^3P)^2P_{1/2}^0$
1625.406	300	61 523.09	-0.003	$(^3F)^4F_{3/2}-(^3P)^4D_{7/2}^0$
1623.067	20	61 611.75	-0.003	$(^3P)^4P_{1/2}-(^3P)^2P_{1/2}^0$
1617.950	300	61 806.60	0.001	$(^3F)^4F_{5/2}-(^3P)^4D_{3/2}^0$
1615.298	20	61 908.08	-0.002	$(^3F)^4F_{5/2}-(^1D)^2F_{9/2}^0$
1615.186	20	61 912.37	0.005	$(^3F)^4F_{3/2}-(^1D)^2P_{3/2}^0$
1610.788	200	62 081.41	-0.004	$(^3F)^4F_{7/2}-(^3P)^4D_{3/2}^0$
1606.711	50	62 238.94	0.002	$(^3F)^4F_{7/2}-(^1D)^2F_{9/2}^0$
1604.734	100	62 315.62	0.001	$(^1D)^2D_{3/2}-(^1G)^2F_{9/2}^0$
1603.342	200	62 369.72	0.004	$(^3F)^4F_{9/2}-(^3P)^4D_{7/2}^0$
1600.200	10	62 492.18	-0.001	$(^3P)^4P_{1/2}-(^3P)^2P_{3/2}^0$
1599.442	200	62 521.80	-0.001	$(^3F)^2F_{5/2}-(^3P)^2D_{3/2}^0$
1599.069	100	62 536.38	0.004	$(^3F)^4F_{3/2}-(^3P)^4D_{5/2}^0$
1594.521	20	62 714.75	0.003	$(^3P)^4P_{5/2}-(^1G)^2F_{9/2}^0$
1588.500	10	62 952.47	0.004	$(^3F)^4F_{9/2}-(^1G)^2G_{9/2}^0$
1586.270	20	63 040.97	0.001	$(^3F)^2F_{5/2}-(^3P)^2D_{3/2}^0$
1583.192	200	63 163.53	0.001	$(^3F)^4F_{5/2}-(^3P)^4D_{3/2}^0$
1572.511	5	63 592.56	0.005	$(^3F)^2F_{7/2}-(^1G)^2F_{9/2}^0$
1570.300	20	63 682.09	0.006	$(^3F)^4F_{9/2}-(^1G)^2G_{7/2}^0$
1569.672	50	63 707.57	0.006	$(^3F)^4F_{7/2}-(^3P)^4D_{9/2}^0$
1566.281	5	63 845.50	-0.004	$(^3F)^4F_{3/2}-(^1F)^2P_{1/2}^0$
1565.110	10	63 893.27	0.005	$(^3F)^4F_{3/2}-(^3P)^4D_{3/2}^0$
1562.312	100	64 007.70	0.011	$(^3F)^4F_{7/2}-(^1D)^2D_{3/2}^0$
1555.451	50	64 290.03	0.013	$(^3F)^4F_{7/2}-(^1G)^2G_{9/2}^0$
1543.457	10	64 789.62	0.012	$(^3F)^4F_{5/2}-(^3P)^4D_{3/2}^0$
1536.944	100	65 064.17	0.006	$(^3F)^2F_{5/2}-(^3P)^2P_{3/2}^0$
1536.333	2	65 090.05	0.009	$(^3F)^4F_{5/2}-(^1D)^2D_{3/2}^0$
1530.300	5	65 346.66	0.006	$(^3F)^4F_{3/2}-(^1D)^2D_{3/2}^0$
1525.431	50	65 555.24	-0.005	$(^3F)^4F_{5/2}-(^3P)^4P_{3/2}^0$
1520.391	20	65 772.55	0.010	$(^3F)^2F_{5/2}-(^1G)^2F_{9/2}^0$
1489.292	20	67 146.00	0.008	$(^3F)^2F_{5/2}-(^1G)^2F_{9/2}^0$
1425.103	100	70 170.37	0.001	$(^3P)^2P_{1/2}-(^1S)^2P_{1/2}^0$
1424.811	50	70 184.74	0.000	$^2D_{1,3/2}-(^3F)^4G_{9/2}^0$
1412.367	300	70 803.12	0.008	$(^3F)^4F_{3/2}-(^3P)^2D_{3/2}^0$
1410.339	50	70 904.93	-0.007	$(^3F)^4F_{9/2}-(^1G)^2F_{9/2}^0$
1394.604	2	71 704.94	0.002	$(^3P)^2P_{3/2}-(^1S)^2P_{3/2}^0$
1378.751	5	72 529.41	0.002	$^2D_{1,3/2}-(^3F)^4F_{3/2}^0$
1363.791	10	73 325.01	-0.003	$(^3F)^4F_{5/2}-(^1G)^2F_{9/2}^0$
1337.710	50	74 754.61	-0.003	$^2D_{1,3/2}-(^3F)^2F_{5/2}^0$
1324.892	50	75 477.85	-0.002	$^2D_{1,3/2}-(^3F)^2D_{3/2}^0$
1301.402	10	76 840.20	-0.006	$^2D_{1,5/2}-(^3F)^2F_{7/2}^0$
1292.743	20	77 354.89	0.010	$^2D_{1,3/2}-(^3F)^4D_{3/2}^0$
1287.641	5	77 661.39	0.002	$^2D_{1,5/2}-(^3F)^4D_{3/2}^0$
1285.748	5	77 775.73	0.007	$(^1D)^2D_{5/2}-(^1S)^2P_{3/2}^0$
1275.937	2	78 373.77	-0.003	$^2D_{1,3/2}-(^3F)^2D_{3/2}^0$
1270.936	10	78 682.16	-0.006	$^2D_{1,5/2}-(^3F)^2D_{3/2}^0$
1270.771	1	78 692.38	-0.004	$^2D_{1,3/2}-(^3P)^2S_{1/2}^0$
1269.850	200	78 749.45	-0.016	$(^1D)^2D_{3/2}-(^1S)^2P_{3/2}^0$
1263.304	1	79 157.51	0.006	$^2D_{1,5/2}-(^3F)^4D_{7/2}^0$
1186.049	200	84 313.54	0.018	$^2F_{5/2}-(^3F)^4G_{9/2}^0$
1181.865	1	84 612.03	-0.002	$^2D_{1,5/2}-(^1D)^2F_{9/2}^0$
1162.450	5	86 025.20	0.001	$^2D_{1,5/2}-(^1D)^2F_{9/2}^0$
1155.375	10	86 551.98	0.007	$F_{7/2}-(^3F)^4G_{7/2}^0$
1153.939	1	86 659.69	-0.001	$^2F_{5/2}-(^3F)^4F_{3/2}^0$
1149.263	5	87 012.28	0.005	$^2D_{1,3/2}-(^1D)^2D_{3/2}^0$
1138.636	5	87 824.37	0.006	$^2F_{5/2}-(^3F)^4F_{3/2}^0$
1115.973	5	89 607.90	-0.001	$^2F_{5/2}-(^3F)^2D_{3/2}^0$
1103.004	1	90 661.50	0.003	$^2F_{5/2}-(^3F)^2F_{9/2}^0$
1099.201	200	90 975.17	-0.001	$^2F_{7/2}-(^3F)^2F_{9/2}^0$

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification 4d ³ , 4d ² (⁵ S-4d ²)(⁵ P)
1093.909	10	91 483.77	-0.004	² F _{5/2} -(³ F) ⁴ D _{5/2} ⁰
1089.364	10	91 796.68	0.001	² F _{7/2} -(³ F) ⁴ D _{5/2} ⁰
1083.330	10	92 307.97	-0.001	² D _{3/2} -(³ F) ⁴ G _{5/2} ⁰
1081.441	20	92 469.21	0.001	² D _{1_{3/2}} -(³ P) ² D _{3/2} ⁰
1079.843	5	92 606.05	-0.001	² D _{2_{3/2}} -(³ F) ⁴ G _{5/2} ⁰
1077.849	50	92 777.37	0.002	² D _{1_{5/2}} -(³ P) ² D _{3/2} ⁰
1077.389	20	92 816.98	0.001	² F _{7/2} -(³ F) ² D _{5/2} ⁰
1075.401	20	92 988.56	0.000	² D _{1_{3/2}} -(³ P) ² D _{5/2} ⁰
1071.885	20	93 293.59	-0.005	² F _{7/2} -(³ F) ⁴ D _{7/2} ⁰
1071.852	100	93 296.46	0.004	² D _{1_{5/2}} -(³ P) ² D _{5/2} ⁰
1064.940	50	93 902.00	-0.001	² F _{5/2} -(³ F) ² G _{7/2} ⁰
1062.343	100	94 131.55	-0.001	² D _{1_{3/2}} -(³ P) ² P _{1/2} ⁰
1057.859	20	94 530.55	-0.004	² D _{2_{5/2}} -(³ F) ⁴ G _{7/2} ⁰
1056.489	1	94 653.13	-0.005	² D _{2_{3/2}} -(³ F) ⁴ F _{3/2} ⁰
1052.495	50	95 012.32	-0.004	² D _{1_{3/2}} -(³ P) ² P _{3/2} ⁰
1049.982	50	95 239.72	-0.001	² P _{3/2} -(³ F) ⁴ G _{5/2} ⁰
1049.096	100	95 320.16	0.001	² D _{1_{5/2}} -(³ P) ² P _{3/2} ⁰
1043.642	1	95 818.29	-0.004	² D _{2_{3/2}} -(³ F) ⁴ F _{5/2} ⁰
1043.206	50	95 858.34	-0.004	² F _{7/2} -(³ F) ² G _{9/2} ⁰
1041.352	100	96 029.00	-0.003	² D _{1_{5/2}} -(¹ G) ² F _{7/2} ⁰
1040.406	50	96 116.32	-0.004	² D _{2_{5/2}} -(³ F) ⁴ F _{5/2} ⁰
1030.018	10	97 085.68	-0.001	² H _{11/2} -(³ F) ² G _{9/2} ⁰
1029.926	100	97 094.35	-0.004	² D _{1_{3/2}} -(¹ G) ² F _{5/2} ⁰
1029.060	50	97 176.06	-0.004	² D _{2_{5/2}} -(³ F) ² F _{5/2} ⁰
1026.671	20	97 402.18	0.000	² D _{1_{3/2}} -(¹ G) ² F _{5/2} ⁰
1026.558	20	97 412.90	-0.006	² P _{1/2} -(³ F) ⁴ F _{3/2} ⁰
1024.740	100	97 585.72	-0.014	² P _{3/2} -(³ F) ⁴ F _{3/2} ⁰
1024.576	20	97 601.34	-0.005	² D _{2_{3/2}} -(³ F) ² D _{3/2} ⁰
1022.465	2	97 802.85	0.004	⁴ P _{5/2} -(³ F) ⁴ G _{5/2} ⁰
1022.336	1	97 815.20	0.000	² D _{2_{5/2}} -(³ F) ⁴ F _{7/2} ⁰
1022.127	50	97 835.20	-0.005	² G _{7/2} -(³ F) ⁴ G _{5/2} ⁰
1015.908	100	98 434.11	-0.003	² F _{5/2} -(¹ D) ² F _{5/2} ⁰
1013.891	10	98 629.93	-0.006	² H _{9/2} -(³ F) ⁴ F _{7/2} ⁰
1012.659	100	98 749.92	-0.003	² P _{3/2} -(³ F) ⁴ F _{5/2} ⁰
1010.574	200	98 953.66	-0.008	² D _{2_{5/2}} -(³ F) ² F _{7/2} ⁰
1009.797	50	99 029.80	-0.011	² G _{9/2} -(³ F) ⁴ G _{7/2} ⁰
1009.225	5	99 085.93	-0.013	⁴ P _{3/2} -(³ F) ⁴ G _{5/2} ⁰
1005.259	200	99 476.85	-0.004	² D _{2_{3/2}} -(³ F) ⁴ D _{5/2} ⁰
1003.965	100	99 605.06	-0.006	² H _{11/2} (³ F) ⁴ F _{9/2} ⁰
1003.106	10	99 690.36	-0.010	² F _{5/2} -(³ P) ² D _{5/2} ⁰
1002.413	1	99 759.28	-0.003	² G _{7/2} -(³ F) ⁴ G _{7/2} ⁰
1002.326	5	99 767.94	-0.009	² H _{9/2} -(³ F) ² F _{7/2} ⁰
1002.245	20	99 776.00	0.007	² D _{2_{5/2}} -(³ F) ⁴ D _{5/2} ⁰
1001.903	200	99 810.06	-0.007	² P _{3/2} -(³ F) ² F _{5/2} ⁰
1001.521	10	99 848.13	-0.010	² F _{5/2} -(¹ D) ² F _{5/2} ⁰
1000.325	3	99 967.51	-0.007	² H _{9/2} -(³ F) ⁴ F _{9/2} ⁰
998.391	100	100 161.15	-0.007	² F _{7/2} -(¹ D) ² F _{7/2} ⁰
996.400	200	100 361.30	-0.008	² P _{1/2} (³ F) ² D _{3/2} ⁰
995.050	200	100 497.46	-0.007	² D _{2_{3/2}} -(³ F) ² D _{5/2} ⁰
994.695	100	100 533.32	-0.007	² P _{3/2} -(³ F) ² D _{3/2} ⁰
992.106	200	100 795.68	-0.009	² D _{2_{5/2}} -(³ F) ² D _{5/2} ⁰
991.907	100	100 815.90	-0.006	² D _{2_{3/2}} -(³ P) ² S _{1/2} ⁰
998.789	20	101 132.89	-0.007	² G _{9/2} -(³ F) ⁴ G _{9/2} ⁰
998.693	5	101 143.63	-0.008	² F _{5/2} -(¹ D) ² D _{3/2} ⁰
987.444	200	101 271.56	-0.007	² D _{2_{5/2}} -(³ F) ⁴ D _{7/2} ⁰
987.011	100	101 315.99	-0.001	² F _{5/2} -(³ P) ⁴ D _{7/2} ⁰
986.722	10	101 345.66	-0.010	² G _{7/2} -(³ F) ⁴ F _{5/2} ⁰
985.900	20	101 430.16	-0.007	⁴ P _{3/2} -(³ F) ⁴ F _{5/2} ⁰
981.065	100	101 930.04	-0.004	² F _{7/2} -(¹ D) ² D _{5/2} ⁰
979.605	2	102 081.96	-0.011	² F _{5/2} -(³ P) ⁴ P _{3/2} ⁰
979.570	10	102 085.60	-0.005	² H _{9/2} -(³ F) ⁴ D _{9/2} ⁰
978.353	100	102 212.59	-0.005	² F _{7/2} -(¹ G) ² G _{9/2} ⁰
978.104	100	102 238.61	-0.003	² P _{1/2} -(³ F) ⁴ D _{3/2} ⁰
976.822	2	102 372.79	0.002	⁴ P _{5/2} -(³ F) ² F _{5/2} ⁰
976.520	100	102 404.45	0.000	² G _{7/2} -(³ F) ² F _{5/2} ⁰
976.466	100	102 410.12	0.002	² P _{3/2} -(³ F) ⁴ D _{3/2} ⁰

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification 4d ³ , 4d ² (⁵ S)-4d ² (⁵ P)
974.710	100	102 594.61	0.000	⁴ P _{3/2} -(³ F) ⁴ F _{5/2} ⁰
974.390	50	102 628.31	0.000	² F _{5/2} -(¹ G) ² G _{7/2} ⁰
971.424	50	102 941.66	0.001	² F _{7/2} -(¹ G) ² G _{7/2} ⁰
970.808	200	103 006.98	0.002	² H _{9/2} -(³ F) ² G _{7/2} ⁰
970.756	50	103 012.49	0.000	⁴ P _{5/2} -(³ F) ⁴ F _{7/2} ⁰
970.456	2	103 044.34	-0.004	² G _{7/2} -(³ F) ⁴ F _{7/2} ⁰
966.851	100	103 428.55	-0.001	² P _{3/2} -(³ F) ² D _{5/2} ⁰
966.638	200	103 451.34	0.000	² G _{9/2} -(³ F) ² F _{7/2} ⁰
965.487	200	103 574.67	0.002	² P _{1/2} -(³ P) ² S _{1/2} ⁰
964.782	20	103 650.35	0.007	² G _{9/2} -(³ F) ⁴ F _{9/2} ⁰
964.748	50	103 654.01	0.004	⁴ P _{3/2} -(³ F) ² F _{5/2} ⁰
963.885	200	103 746.81	0.002	² P _{3/2} -(³ P) ² S _{1/2} ⁰
961.404	50	104 014.54	-0.004	² D _{2_{5/2}} -(³ P) ⁴ S _{3/2} ⁰
960.520	100	104 110.27	0.004	² F _{7/2} -(³ P) ⁴ P _{5/2} ⁰
960.147	200	104 150.71	-0.005	⁴ P _{5/2} -(³ F) ² F _{7/2} ⁰
958.887	300	104 287.57	0.000	² H _{11/2} -(³ F) ² G _{9/2} ⁰
958.130	50	104 369.97	0.003	⁴ P _{1/2} -(³ F) ² D _{3/2} ⁰
958.058	50	104 377.81	-0.002	⁴ P _{3/2} -(³ F) ² D _{3/2} ⁰
955.568	100	104 649.80	0.001	² H _{9/2} -(³ F) ² G _{9/2} ⁰
952.633	100	104 972.21	-0.004	⁴ P _{5/2} -(³ F) ⁴ D _{5/2} ⁰
952.348	100	105 003.63	-0.003	² G _{7/2} -(³ F) ⁴ D _{5/2} ⁰
949.109	20	105 361.97	0.003	² F _{7/2} -(¹ G) ² H _{9/2} ⁰
948.304	100	105 451.41	0.000	⁴ P _{1/2} -(³ F) ⁴ D _{5/2} ⁰
948.244	10	105 458.08	0.006	⁴ P _{3/2} -(³ F) ⁴ D _{1/2} ⁰
945.556	10	105 769.06	0.003	² G _{9/2} -(³ F) ² D _{7/2} ⁰
943.463	50	105 992.49	-0.004	⁴ P _{5/2} -(³ F) ² D _{5/2} ⁰
943.403	100	105 999.23	0.003	² D _{2_{5/2}} -(¹ D) ² P _{3/2} ⁰
943.187	50	106 023.51	0.000	² G _{7/2} -(³ F) ² D _{5/2} ⁰
941.194	50	106 248.02	0.000	⁴ P _{1/2} -(³ F) ⁴ D _{3/2} ⁰
941.143	100	106 253.77	-0.005	⁴ P _{3/2} -(³ F) ⁴ D _{5/2} ⁰
939.617	50	106 426.34	0.004	² D _{3/2} -(¹ D) ² F _{5/2} ⁰
939.242	200	106 468.83	-0.006	⁴ P _{5/2} -(³ F) ⁴ D _{7/2} ⁰
938.092	200	106 599.35	0.001	² F _{5/2} -(³ P) ² D _{3/2} ⁰
937.881	100	106 623.33	0.002	² D _{2_{5/2}} -(³ P) ⁴ D _{3/2} ⁰
937.668	20	106 647.55	0.003	² P _{3/2} -(³ P) ⁴ S _{3/2} ⁰
937.285	200	106 691.13	0.003	² G _{9/2} -(³ F) ² G _{9/2} ⁰
936.993	50	106 724.38	0.004	² D _{2_{5/2}} -(¹ D) ² F _{5/2} ⁰
933.548	10	107 118.22	0.004	² F _{5/2} -(³ P) ² D _{5/2} ⁰
932.200	10	107 273.11	0.003	⁴ P _{3/2} -(³ F) ² D _{5/2} ⁰
931.185	5	107 390.04	0.003	⁴ P _{3/2} -(³ F) ² G _{7/2} ⁰
930.911	300	107 421.65	0.001	² G _{7/2} -(³ F) ² G _{9/2} ⁰
930.822	300	107 431.92	0.001	² F _{7/2} -(³ P) ² D _{5/2} ⁰
929.493	10	107 585.53	-0.008	⁴ P _{1/2} -(³ P) ² S _{1/2} ⁰
929.437	100	107 592.01	0.000	⁴ P _{3/2} -(³ P) ² S _{1/2} ⁰
929.072	200	107 634.28	0.000	² D _{2_{5/2}} -(¹ D) ² P _{1/2} ⁰
928.895	2	107 654.79	0.006	⁴ F _{7/2} -(³ F) ⁴ G _{5/2} ⁰
926.099	10	107 979.81	0.005	² D _{2_{5/2}} -(³ P) ⁴ D _{5/2} ⁰
924.748	5	108 137.56	0.006	² D _{2_{5/2}} -(¹ D) ² F _{7/2} ⁰
923.072	300	108 333.91	0.003	² G _{9/2} -(³ F) ² G _{9/2} ⁰
921.997	20	108 460.22	0.008	² P _{1/2} -(¹ D) ² P _{3/2} ⁰
921.874	10	108 474.69	0.002	⁴ F _{9/2} -(³ F) ⁴ G _{7/2} ⁰
920.529	200	108 633.18	0.000	² P _{3/2} -(¹ D) ² P _{3/2} ⁰
917.837	10	108 951.80	0.005	² H _{9/2} -(¹ D) ² F _{7/2} ⁰
916.891	50	109 064.21	0.002	² G _{7/2} -(<

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification
907.745	200	110 163.09	0.008	² F _{7/2} -(¹ G) ² F ^{07/2}
906.034	20	110 371.13	0.006	² D _{5/2} -(³ P) ⁴ P ⁰ _{3/2}
905.853	100	110 393.18	0.006	² P _{1/2} -(¹ D) ² P ⁰ _{1/2}
905.630	200	110 420.37	0.007	² H _{9/2} -(³ P) ⁴ D ⁰ _{7/2}
905.102	200	110 484.78	0.006	⁴ P _{1/2} -(³ P) ⁴ S ⁰ _{3/2}
905.038	200	110 492.59	0.002	⁴ P _{3/2} -(³ P) ⁴ S ⁰ _{3/2}
904.487	300	110 559.90	-0.003	⁴ F _{5/2} -(³ F) ⁴ G ⁰ _{5/2}
904.337	100	110 578.24	0.002	⁴ F _{9/2} -(³ F) ⁴ G ⁰ _{9/2}
904.047	50	110 613.71	0.003	² P _{3/2} -(³ P) ⁴ D ⁰ _{3/2}
903.821	300	110 641.37	0.002	² H _{11/2} -(¹ G) ² G ⁰ _{9/2}
902.220	200	110 837.71	0.008	² D _{13/2} -(¹ S) ² P ⁰ _{1/2}
901.559	10	110 918.97	0.004	² D _{5/2} -(¹ G) ² G ⁰ _{7/2}
900.873	100	111 003.43	0.004	² H _{9/2} -(¹ G) ² G ⁰ _{9/2}
899.563	10	111 165.08	0.003	⁴ F _{7/2} -(³ F) ⁴ F ⁰ _{5/2}
899.306	100	111 196.85	0.000	⁴ P _{5/2} -(¹ D) ² P ⁰ _{3/2}
899.093	200	111 223.19	0.007	² F _{5/2} -(¹ G) ² F ⁰ _{5/2}
895.391	200	111 683.05	0.002	⁴ F _{7/2} -(³ F) ⁴ G ⁰ _{5/2}
894.992	200	111 732.84	0.007	² H _{9/2} -(¹ G) ² G ⁰ _{7/2}
894.774	200	111 760.06	{ -0.001 -0.001	{ ⁴ F _{9/2} -(³ F) ⁴ F ⁰ _{7/2} ⁴ F _{3/2} -(³ F) ⁴ F ⁰ _{3/2}
894.537	5	111 789.67	0.006	² D _{3/2} -(³ P) ⁴ P ⁰ _{3/2}
894.289	30	111 820.67	0.001	⁴ P _{5/2} -(³ P) ⁴ D ⁰ _{3/2}
893.234	200	111 952.74	0.007	² G _{7/2} -(¹ D) ² F ⁰ _{3/2}
892.211	50	112 081.11	0.001	⁴ P _{1/2} -(³ P) ⁴ D ⁰ _{1/2}
892.154	100	112 088.27	{ 0.002 0.003	{ ² D _{5/2} -(³ P) ⁴ P ⁰ _{3/2} ⁴ P _{3/2} -(³ P) ⁴ D ⁰ _{1/2}
891.704	200	112 144.83	0.003	⁴ F _{5/2} -(³ F) ⁴ F ⁰ _{3/2}
891.065	100	112 225.25	0.000	⁴ F _{7/2} -(³ F) ⁴ F ⁰ _{5/2}
889.066	50	112 477.58	0.005	⁴ P _{3/2} -(¹ D) ² P ⁰ _{3/2}
888.571	5	112 540.24	0.006	² P _{3/2} -(¹ D) ² D ⁰ _{5/2}
888.225	20	112 584.08	0.006	² P _{3/2} -(³ P) ⁴ P ⁰ _{1/2}
887.813	300	112 636.33	0.003	² G _{9/2} -(¹ D) ² F ⁰ _{7/2}
886.269	10	112 832.56	0.007	² P _{1/2} -(³ P) ⁴ P ⁰ _{3/2}
886.015	400	112 864.90	-0.001	⁴ F _{7/2} -(³ F) ⁴ F ⁰ _{7/2}
885.760	200	112 897.39	0.001	⁴ F _{9/2} -(³ F) ⁴ F ⁰ _{7/2}
885.540	100	112 925.44	-0.002	⁴ F _{3/2} -(³ F) ⁴ F ⁰ _{5/2}
884.919	10	113 004.69	0.007	² P _{3/2} -(³ P) ⁴ P ⁰ _{3/2}
884.830	200	113 016.06	0.004	⁴ F _{9/2} -(³ F) ⁴ G ⁰ _{11/2}
884.195	500	113 097.22	0.001	⁴ F _{9/2} -(³ F) ⁴ F ⁰ _{9/2}
883.564	5	113 177.99	-0.002	⁴ P _{5/2} -(³ P) ⁴ D ⁰ _{5/2}
883.361	200	113 204.00	{ -0.003 0.007	{ ⁴ P _{3/2} -(¹ D) ² F ⁰ _{3/2} ⁴ F _{5/2} -(³ F) ⁴ F ⁰ _{5/2}
883.321	200	113 209.12	0.000	² G _{7/2} -(³ P) ⁴ D ⁰ _{5/2}
882.338	50	113 335.25	0.002	⁴ P _{5/2} -(¹ D) ² F ⁰ _{7/2}
882.093	100	113 366.73	0.002	² G _{7/2} -(¹ D) ² F ⁰ _{7/2}
880.853	20	113 526.32	0.003	² D _{13/2} -(¹ S) ² P ⁰ _{3/2}
878.801	100	113 791.40	0.003	² H _{11/2} -(¹ G) ² H ⁰ _{9/2}
878.474	100	113 833.76	0.009	² D _{15/2} -(¹ S) ² P ⁰ _{3/2}
878.394	100	113 844.12	0.003	⁴ F _{5/2} -(³ F) ⁴ F ⁰ _{7/2}
877.750	200	113 927.65	0.004	⁴ F _{3/2} -(³ F) ⁴ P ⁰ _{3/2}
877.308	10	113 985.05	-0.001	⁴ F ₃ -(³ F) ² F ⁰ _{5/2}
876.384	100	114 105.23	0.002	² G _{9/2} -(³ P) ⁴ D ⁰ _{7/2}
876.013	200	114 153.55	0.005	² H _{9/2} -(¹ G) ² H ⁰ _{9/2}
875.642	50	114 201.92	0.002	⁴ F _{7/2} -(³ F) ⁴ F ⁰ _{9/2}
874.047	10	114 410.32	0.005	⁴ P _{3/2} -(¹ D) ² P ⁰ _{1/2}
873.676	100	114 458.90	0.002	⁴ P _{3/2} -(³ P) ⁴ D ⁰ _{5/2}
872.362	20	114 631.31	-0.001	⁴ P _{5/2} -(¹ D) ² D ⁰ _{3/2}
871.933	100	114 687.71	0.004	² G _{9/2} -(¹ G) ² G ⁰ _{9/2}
871.777	50	114 708.23	0.000	⁴ F _{3/2} -(³ F) ² D ⁰ _{3/2}

Table I. Continued

Wavelength (Å)	Int.	Wavenumber (cm ⁻¹)	O-C (Å)	Classification
871.677	50	114 721.39	0.006	² P _{3/2} -(³ P) ⁴ P ⁰ _{5/2}
871.052	100	114 803.70	0.005	⁴ P _{5/2} -(³ P) ⁴ D ⁰ _{7/2}
870.899	200	114 823.87	0.001	⁴ F _{7/2} -(³ F) ⁴ D ⁰ _{5/2}
870.813	100	114 835.21	0.004	² G _{7/2} -(³ P) ⁴ D ⁰ _{7/2}
870.394	10	114 890.49	0.000	² D _{5/2} -(³ P) ² D ⁰ _{3/2}
868.774	100	115 104.73	-0.001	⁴ P _{5/2} -(¹ D) ² D ⁰ _{5/2}
868.539	50	115 135.87	0.001	² G _{7/2} -(¹ D) ² D ⁰ _{5/2}
867.941	300	115 215.20	0.003	⁴ F _{9/2} -(³ F) ⁴ D ⁰ _{7/2}
866.418	100	115 417.73	{ 0.002 0.006	{ ² G _{9/2} -(¹ G) ² G ⁰ _{9/2} ² G _{7/2} -(¹ G) ² G ⁰ _{9/2}
865.284	100	115 568.99	0.002	⁴ P _{5/2} -(³ P) ⁴ P ⁰ _{3/2}
864.647	300	115 654.13	0.006	² H _{11/2} -(¹ G) ² H ⁰ _{11/2}
863.636	200	115 789.52	-0.001	⁴ F _{7/2} -(³ F) ⁴ D ⁰ _{1/2}
863.515	200	115 805.74	0.002	⁴ F _{5/2} -(³ F) ⁴ D ⁰ _{3/2}
863.228	200	115 844.25	0.001	⁴ F _{7/2} -(³ F) ² D ⁰ _{5/2}
862.775	5	115 905.07	0.001	⁴ P _{1/2} -(¹ D) ² D ⁰ _{3/2}
861.203	5	116 116.64	0.001	⁴ P _{5/2} -(¹ G) ² G ⁰ _{7/2}
861.054	50	116 136.73	0.008	⁴ F _{9/2} -(³ F) ² G ⁰ _{7/2}
860.187	50	116 253.79	0.006	² D _{3/2} -(³ P) ² F ⁰ _{1/2}
859.695	50	116 320.32	0.001	⁴ F _{7/2} -(³ F) ² D ⁰ _{1/2}
859.211	20	116 385.84	0.001	⁴ P _{3/2} -(¹ D) ² D ⁰ _{3/2}
858.937	10	116 422.97	-0.004	⁴ P _{1/2} -(³ P) ⁴ P ⁰ _{1/2}
858.886	100	116 429.88	0.000	⁴ P _{3/2} -(³ P) ⁴ P ⁰ _{1/2}
857.734	100	116 586.26	-0.002	⁴ F _{3/2} -(³ F) ⁴ D ⁰ _{3/2}
855.984	100	116 824.61	-0.004	⁴ F _{5/2} -(³ F) ² D ⁰ _{5/2}
855.849	100	116 843.04	0.001	⁴ P _{1/2} -(³ P) ⁴ P ⁰ _{3/2}
855.795	5	116 850.41	0.001	⁴ P _{3/2} -(³ P) ⁴ P ⁰ _{3/2}
853.718	100	117 134.69	0.003	² D _{3/2} -(³ P) ² P ⁰ _{3/2}
852.938	2	117 241.81	0.005	⁴ F _{7/2} -(³ F) ² G ⁰ _{7/2}
852.620	200	117 285.54	0.002	⁴ P _{5/2} -(³ P) ⁴ P ⁰ _{5/2}
852.392	2	117 316.91	0.002	² G _{7/2} -(³ P) ⁴ P ⁰ _{5/2}
851.549	100	117 433.05	0.001	² D _{5/2} -(³ P) ² P ⁰ _{3/2}
850.312	3	117 603.89	0.001	⁴ F _{3/2} -(³ F) ² D ⁰ _{3/2}
849.040	50	117 780.08	0.003	⁴ F _{9/2} -(³ F) ² G ⁰ _{9/2}
846.443	8	118 141.44	0.002	² D _{5/2} -(¹ G) ² F ⁰ _{7/2}
845.865	2	118 222.17	0.001	⁴ F _{5/2} -(³ F) ² G ⁰ _{9/2}
843.404	20	118 567.14	0.000	⁴ P _{3/2} -(³ P) ⁴ P ⁰ _{5/2}
841.145	10	118 885.56	-0.002	⁴ F _{7/2} -(³ F) ² G ⁰ _{9/2}
840.651	20	118 955.42	0.004	² H _{9/2} -(¹ G) ² F ⁰ _{7/2}
840.233	10	119 014.60	-0.002	² P _{1/2} -(³ P) ² P ⁰ _{1/2}
839.024	50	119 186.10	0.002	² P _{3/2} -(³ P) ² P ⁰ _{1/2}
838.809	5	119 216.65	0.003	² D _{3/2} -(¹ G) ² F ⁰ _{3/2}
835.410	50	119 701.70	-0.001	² G _{9/2} -(¹ G) ² H ⁰ _{11/2}
821.189	1	121 774.64	-0.001	⁴ F _{7/2} -(¹ D) ² F ⁰ _{5/2}
819.471	2	122 029.94	-0.008	⁴ F _{5/2} -(¹ D) ² P ⁰ _{3/2}
819.110	5	122 083.72	-0.005	⁴ F _{9/2} -(¹ D) ² F ⁰ _{7/2}
816.856	20	122 420.59	-0.009	⁴ F _{3/2} -(³ P) ⁴ D ⁰ _{1/2}
815.386	1	122 641.30	-0.007	² G _{9/2} -(¹ G) ² F ⁰ _{7/2}
815.305	50	122 653.48	-0.005	⁴ F _{5/2} -(³ P) ⁴ D ⁰ _{3/2}
812.801	100	123 031.34	{ -0.009 0.000	{ ⁴ F _{7/2} -(³ P) ⁴ D ⁰ _{3/2} ⁴ P _{3/2} -(³ P) ² P ⁰ _{1/2}
810.152	2	123 433.62	-0.006	⁴ F _{3/2} -(³ P) ⁴ D ⁰ _{3/2}
809.369	100	123 533.03	-0.008	⁴ F _{9/2} -(³ P) ⁴ D ⁰ _{7/2}
806.387	10	124 009.93	-0.001	⁴ F _{5/2} -(³ P) ⁴ D ⁰ _{5/2}
805.362	20	124 167.76	-0.002	⁴ F _{5/2} -(¹ D) ² F ⁰ _{7/2}
802.200	2	124 657.19	-0.004	⁴ F _{7/2} -(³ P) ⁴ D ⁰ _{7/2}
801.639	2	124 744.43	-0.004	² G _{7/2} -(¹ G) ² F ⁰ _{5/2}
800.858	2	124 866.08	-0.01	

Table II. Even levels of triply ionized molybdenum (Mo IV). The level, level uncertainty and O-C values are given in units of cm^{-1} . The number of transitions to each level is given in the column headed "No". The "Leading Percentages" are given in LS coupling

Config.	Term	J	Level	Unc.	No.	O-C	Leading percentages
$4d^3$	4F	3/2	0.00	0.25	10	-10	99
		5/2	778.02	0.26	12	-10	100
		7/2	1 759.76	0.22	16	-10	100
		9/2	2 864.58	0.27	12	0	98
$4d^3$	4P	1/2	10 337.77	0.30	10	0	93
		3/2	10 330.59	0.19	20	20	83 14^3P
		5/2	11 611.99	0.16	19	20	99
$4d^3$	2G	7/2	11 580.50	0.17	17	-20	99
		9/2	12 310.80	0.24	13	0	83 15^2H
$4d^3$	2P	3/2	14 175.62	0.21	17	20	45 31^2D_2 , 15^4P
		1/2	14 347.72	0.30	8	60	93
$4d^3$	2H	9/2	15 995.13	0.26	12	20	85 15^2G
		11/2	16 357.48	0.29	6	30	100
$4d^3$	2D_2	5/2	16 809.32	0.15	24	-60	81 17^2D_1
		3/2	17 107.35	0.19	16	0	43 41^2P , 13^2D_1
$4d^3$	2F	7/2	24 787.03	0.17	14	-30	99
		5/2	25 100.40	0.20	19	-30	99
$4d^3$	2D_1	5/2	38 922.29	0.14	12	30	81 16^2D_2
		3/2	39 230.53	0.12	15	-20	77 23^2D_2
$4d^2(^3F)5s$	4F	3/2	60 896.28	0.07	17	20	99
		5/2	61 626.19	0.05	21	10	98
		7/2	62 708.50	0.06	18	10	99
		9/2	64 046.46	0.07	12	0	100
$4d^2(^3F)5s$	2F	5/2	69 178.07	0.05	25	-30	94
		7/2	71 358.31	0.05	20	-10	98
$4d^2(^3P)5s$	4P	1/2	71 750.36	0.06	12	-10	100
		3/2	72 162.82	0.05	17	-10	93
		5/2	72 236.20	0.06	16	-30	70 $27(^1D)2D$
$4d^2(^1D)5s$	2D	3/2	74 008.77	0.04	24	10	89 $7(^3P)4P$
		5/2	74 981.08	0.04	17	-10	68 $29(^3P)4P$
$4d^2(^1G)5s$	2G	9/2	79 106.26	0.05	9	-20	100
		7/2	79 193.56	0.05	10	20	99
$4d^2(^3P)5s$	2P	1/2	79 898.80	0.05	9	20	99
		3/2	81 052.21	0.05	13	20	96
$4d^2(^1S)5s$	2S	1/2	99 783.80	0.08	3	0	99

 Table III. Odd levels of triply ionized molybdenum (Mo IV). The level, level uncertainty and O-C values are given in units of cm^{-1} . The number of transitions from each level is given in the column headed "No"

Config.	Term	J	Level	Unc.	No.	O-C	Leading Percentages
$4d^2(^3F)5p$	4G	5/2	109 415.25	0.06	14	-140	82 $12(^3F)^2F$
		7/2	111 339.53	0.06	12	-100	90
		9/2	113 443.02	0.07	7	-80	92
		11/2	115 881.12	0.15	2	-60	100
$4d^2(^3F)5p$	4F	3/2	111 760.03	0.05	12	110	75 $19(^3F)^2D$
		5/2	112 925.24	0.05	16	0	73 $12(^3F)^2D$ $7(^3F)^4D$
		7/2	114 624.49	0.09	11	90	90
		9/2	115 961.91	0.07	9	100	82 $8(^3F)^4G$
$4d^2(^3F)5p$	2F	5/2	113 984.98	0.05	16	-120	41 $19(^3F)^4F$ $16(^3F)^4G$
		7/2	115 762.16	0.05	15	-110	61 $25(^3F)^4D$ $6(^3F)^4G$
$4d^2(^3F)5p$	2D	3/2	114 708.24	0.07	16	-60	42 $23(^3F)^4F$ $17(^3F)^4D$
		5/2	117 604.08	0.05	20	-120	32 $26(^3F)^4D$ $18(^3P)^2D$
$4d^2(^3F)5p$	4D	1/2	115 789.36	0.11	5	100	79 $17(^3P)^4D$
		3/2	116 586.00	0.09	12	0	60 $17(^3P)^4D$ $13(^3F)^2D$
		5/2	116 583.82	0.06	15	-70	47 $19(^3F)^2F$ $13(^3F)^2D$
		7/2	118 080.17	0.09	13	-60	55 $19(^3F)^2F$ $10(^3P)^4D$

Table III. Continued

Config.	Term	J	Level	Unc.	No.	$O-C$	Leading Percentages
$4d^2(^3P)5p$	2S	1/2	117922.63	0.08	10	-40	92
$4d^2(^3F)5p$	2G	7/2	119002.33	0.10	14	210	78 $12(^1G)^2G$
		9/2	120645.02	0.10	11	150	73 $14(^1G)^2G$ $11(^3F)^4F$
$4d^2(^3P)5p$	4S	3/2	120823.46	0.08	11	-240	65 $25(^1D)^2P$
$4d^2(^3P)5p$	4D	1/2	122419.26	0.08	7	60	80 $18(^3F)^4D$
		3/2	123432.84	0.08	14	-60	49 $27(^1D)^2P$ $12(^3P)^4S$
		5/2	124789.75	0.06	16	110	69 $15(^1D)^2F$ $10(^3F)^4D$
		7/2	126416.33	0.09	16	80	54 $31(^1G)^2G$ $5(^3F)^2G$
$4d^2(^1D)5p$	2P	3/2	122808.84	0.12	12	-90	19 $31(^3P)^4D$ $19(^3P)^4S$
		1/2	124741.62	0.09	7	-230	79 $16(^3P)^4P$
$4d^2(^1D)5p$	2F	5/2	123534.18	0.06	14	280	61 $13(^3F)^2F$ $7(^3P)^4D$
		7/2	124947.54	0.07	17	160	45 $18(^1G)^2G$ $18(^3P)^4D$
$4d^2(^1D)5p$	2D	3/2	126243.19	0.11	14	70	40 $21(^3P)^4P$ $19(^1D)^2P$
		5/2	126716.64	0.09	14	-20	46 $35(^3P)^4P$ $7(^3P)^4D$
$4d^2(^3P)5p$	4P	1/2	126760.46	0.10	8	180	79 $13(^1D)^2P$
		3/2	127181.20	0.09	16	150	75 $19(^1D)^2D$
		5/2	128897.78	0.07	13	-30	59 $38(^1D)^2D$
$4d^2(^1G)5p$	2G	7/2	127728.82	0.08	13	110	35 $33(^1D)^2F$ $17(^3P)^4D$
		9/2	126999.09	0.11	10	90	71 $18(^3F)^2G$ $11(^1G)^2H$
$4d^2(^1G)5p$	2H	9/2	130149.35	0.10	6	120	87 $13(^1G)^2G$
		11/2	132012.37	0.15	3	110	100
$4d^2(^3P)5p$	2D	3/2	131699.83	0.08	12	-60	62 $17(^3P)^2P$ $12(^3F)^2D$
		5/2	132219.07	0.09	9	-30	72 $19(^3F)^2D$
$4d^2(^3P)5p$	2P	1/2	133362.00	0.08	10	50	94
		3/2	134242.50	0.08	12	-30	77 $11(^3P)^2D$ $6(^1D)^2D$
$4d^2(^1G)5p$	2F	7/2	134951.06	0.11	13	-220	91
		5/2	136324.44	0.13	9	-260	95
$4d^2(^1S)5p$	2P	1/2	150069.22	0.14	3	0	94
		3/2	152757.31	0.19	6	0	97

Table IV. LSF and HFR parameter values for the $4d^3$, $4d^25s$ and $4d^25p$ configurations of triply ionized molybdenum (Mo IV) in cm^{-1}

Config.	Parameter	LSF	HRF	LSF/HRF
$4d^3$	E_{av}	14588(10)	-	-
	$F^2(dd)$	50411(37)	63051	0.80
	$F^4(dd)$	32830(77)	41431	0.79
	ζ_d	810(7)	796	1.01
	α	38(2)	-	-
	β	-313(31)	-	-
	$4d^25s$	E_{av}	71732(13)	72375
$F^2(dd)$		52632(62)	65612	0.80
$F^4(dd)$		34979(89)	43294	0.81
ζ_d		878(8)	864	1.02
$G^2(ds)$		12685(64)	15887	0.80
α		33(2)	-	-
β		-339(29)	-	-
C.I.		$R^2(dd, ds)$	-8830(700)	-17415

Standard deviation = 30 cm^{-1}

Table IV. Continued

Config.	Parameter	LSF	HRF	LSF/HRF
$4d^25p$	E_{av}	122801(23)	122387	1.00
	$F^2(dd)$	52890(250)	66044	0.80
	$F^4(dd)$	35460(310)	43614	0.82
	ζ_d	926(23)	873	1.06
	ζ_p	2136(55)	1698	1.26
	$F^2(dp)$	19490(180)	24874	0.78
	$G^1(dp)$	7534(100)	9821	0.77
	$G^3(dp)$	4320(240)	8595	0.50
	α	38(6)	-	-
	β	-240(100)	-	-

Standard deviation = 141 cm^{-1}