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2015 Phys. Scr. 90 095402

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Observation of core-excited configuration in four-time ionized neodymium Nd⁴⁺ (Nd V)

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Received 4 December 2014, revised 10 July 2015

Accepted for publication 17 July 2015

Published 13 August 2015



CrossMark

Abstract

Laboratory observation of the Nd V spectrum has been extended to shorter wavelength region down to 370 Å. The analysis, based on 304 spectral lines led to the determination of 104 energy levels of the core-excited configuration 5p⁵4f²5d. The configuration interaction effects were studied by parametric calculations (Slater–Racah) of the odd-parity configurations where energy parameter values were least-squares fitted against the observed levels, starting with their Hartree-Fock values. The results confirmed the reduction of transition probabilities for the 5p⁶4f²-5p⁶4f5d transitions predicted in the previous Nd V study.

Keywords: atomic spectra, transitions, energy levels, lanthanide ions

(Some figures may appear in colour only in the online journal)

1. Introduction

Spectra and energy levels of lanthanide ions of different ionization stages are basic data of interest in many areas such as plasma diagnostics, material sciences and astrophysics. In astrophysics, singly and doubly charged ions (spectra II and III) are detected in spectra of chemically peculiar stars (see for example reference [1, 2]). In material sciences, triply ionized lanthanide ions (spectra IV) embedded in crystal have long been used in solid state laser materials [3]. These triply charged ions, sometimes together with the four-time charged ions, are also involved in research on thin films (see for example reference [4]). In these solid state cases, data on free ions are references for analyzing influences of the environment on the energy levels or transition probabilities of the embedded ions. Therefore, energy levels and radiative properties of lanthanide free ions are upstream of various applications. The interpretation of laboratory emission spectra resulting in the determination of energy levels of lanthanide free ions is a challenging task, given their complexities, which

can only be achieved by high resolution studies. The reliability of results is greatly supported by comparison of variation trends of energy parameters in isoelectronic or isoionic sequences, or in neighboring ions. Often, several neighboring ionization stages need to be studied at the same time. From the point of view of the theory of atomic structure, the identification of the strongest radiative transitions leads to the knowledge of the ground and low-lying excited configurations in lanthanide ions and provides test cases for theoretical modeling of atomic systems with f shells electrons (see for example reference [5–7]). In the vacuum ultraviolet domain, taking advantage of the high resolution VUV spectrograph of the Meudon Observatory, we undertook the emission study of unknown spectra of lanthanide ions, mainly the fourth and the fifth spectra, which already led to publications on Nd IV [5, 8, 9], Nd V [10] and Tm IV [11]. The fourth spectra have been often investigated because of applications to laser materials, while the fifth spectra are still very incompletely known, although they are relevant for a better description of the fⁿ core in the fourth spectra. Before the first study of Nd V

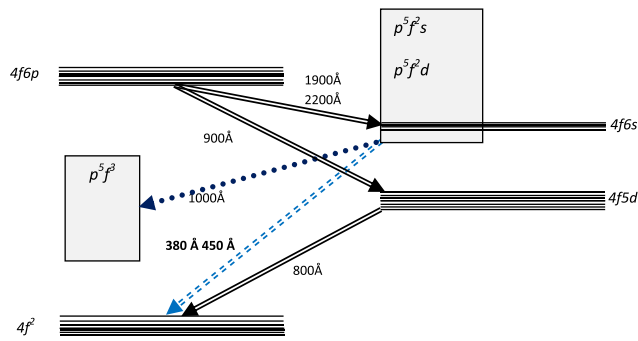


Figure 1. Transition diagram of Nd^{4+} . Solid arrows represent the classified lines in [10], the dashed arrow, those classified in the present work and the dotted arrow is an unknown transition array.

by Meftah *et al* [10], all the fifth lanthanide spectra were unknown except for La V, Ce V, Pr V, and Lu V (See reference in [12]). Only recently Yb V [13] was added to this series.

The Nd^{4+} ion (Nd V) belongs to the barium (Ba I) iso-electronic sequence in which the ground state electronic configurations are built on two valence electrons outside a closed $5p^6$ sub-shell: $6s^2$ in Ba I, $5d^2$ in La II, $4f^2$ in Ce III and Pr IV. Reference on these spectra can be found in [12]. As for Nd V, it was established by Meftah *et al* [10] that the lowest configurations above the ground configuration $4f^2$ are $4f5d$, $4f6s$, $4f6p$ (figure 1). All levels of these configurations (except $4f^2$ 1S_0) were derived [10] from their transitions in the wavelength region 713–2238 Å. Unknown configurations of higher energy in Nd V were investigated theoretically in [10] by the Hartree–Fock method including relativistic corrections and it was obvious that the $5p^64f6s$ configuration would overlap and mix with the core-excited configuration $5p^54f^25d$. Due to the lack of observations in the wavelength range 350–500 Å, where the $5p^64f^2$ – $5p^54f^25d$ transitions were predicted, the core-excited configuration $5p^54f^25d$ could not be localized in [10]. However, the effect of the $5p^64f5d$ – $5p^54f^25d$ configuration interaction (CI) was made clear by a strong reduction of the calculated transition probabilities for the transition array $5p^64f^2$ – $5p^64f5d$. Recently, core-excited configurations $5p^54f5d$ and $5p^54f6s$ were observed and interpreted in Ce IV [14] of the Cs I sequence. Their interaction with the $5p^6nd$ series was invoked for explaining the large fine structure splitting observed in the $6d$ 2D term. This brought another example of interaction between open sub-shell and complete sub-shell configurations. However, generally speaking, core-excited configurations did not receive much attention.

The aim of the present work is to extend the previous analysis of Nd V [10] and to determine the levels of the core excited $5p^54f^25d$ configuration in Nd V from their transitions to the ground configuration by extending the observation of the emission spectrum to a shorter wavelength region and to further investigate the effect of configuration interaction on transition probabilities.

2. Experiment and line list

As described in [10], the previous study of the Nd V spectrum made use of two sets of emission data from sliding spark sources. One was recorded in the wavelength range of 500–2700 Å, some years ago, on the 10.7 m normal incidence spectrograph (1200 lines mm^{-1} concave grating, plate factor 0.78 Å mm^{-1} in the first order) at the National Bureau of Standards (NBS) with photographic plates (PP). The second set was recorded in the range of 700–1000 Å on the 10.7 m vacuum ultraviolet normal incidence spectrograph of the Paris-Meudon Observatory (3600 lines mm^{-1} holographic concave grating, plate factor of 0.26 Å mm^{-1}), either on photographic plates or on phosphor storage image plates (IP). The latter ones were used for intensity measurements because of their linear intensity response over five orders of magnitude. For the present work, the transition arrays of interest were predicted to fall below 500 Å. For a start, we extended measurements of wavelengths down to 393 Å on one spectrum from NBS PP, using impurity lines from C, N, O ions as wavelength references. However, reference lines were scarce below 450 Å, therefore more emission spectra were recorded in Meudon extending the wavelength region to the shorter end. Alternatively a pure neodymium anode and an anode in an Nd/Fe/B alloy were used, in order to produce ionized iron lines for wavelength references. Two types of vacuum spark sources were available. The same sliding spark source as in [10] was used to produce Nd^{4+} emission in the wavelength range of (440–650 Å). In order to increase the energy of discharge, a three-electrode triggered spark source was used for the wavelength range 350–555 Å, in a similar setting as in the W VIII study [15].

Spectra recorded on image plates (Fuji BAS-TR 2040) were digitized by a specific scanner FUJI9000 that has a sample step of 10 microns. However, the photographic spectra from NBS show more lines in the overlap region (450–555 Å). Thus the final line list of table 1 contains classified lines from IP between 370–447 Å and from PP between 447–555 Å, with intensities from IP when available. For wavelength measurements, the photographic spectra were first digitized by a high resolution optical scanner iQsmart1 with correction of possible non-linearities in displacement by simultaneously scanning an optical ruler, as explained in the recent article on Yb V [13]. In the measurement software, an experimental intensity with arbitrary units could be estimated for each line from the area under a triangle fitting the line profile.

For wavelength calibration, reference lines were taken among impurity lines from low Z elements (O and N) [16] and from the newly compiled [17] Ritz wavelengths of Fe V lines present in the emission of the Nd/Fe/B alloy anode. Some Ritz wavelengths of Nd V from the previous study [10] were also used as references. The uncertainty on measured wavelengths can be estimated to be around $\pm 0.005 \text{ Å}$ for isolated lines.

Table 1. Observed lines identified as the $5p^64f^2-5p^54f^25d$ transitions in Nd V. $\Delta\lambda = \lambda_{\text{exp}} - \lambda_{\text{Ritz}}$; intensities in arbitrary units (PP: photographic plates, IP: image plates); calculated transition probabilities gA , g being the statistical weight of the upper level, with a 12-configuration basis. CF is the cancellation factor defined by equation (14.107), p432 in [18]. λ_{Ritz} is derived from the level energies as $\lambda_{\text{Ritz}} = (E_{\text{up}} - E_{\text{low}})^{-1}$. All energies and wave numbers are in cm^{-1} . The comments after the wavelengths and the level labels are explained in footnotes at the end of the table.

λ (Å)	Int _{exp}		gA s^{-1}	CF	σ_{exp} (cm^{-1})	λ_{Ritz} (Å)	$\Delta\lambda$ (Å)	Lower level label	E_{low}	Upper level label	E_{up}
370.698		31	4.19E + 11	0.86	269 761.1	370.698	0.000	p6-f2_3H 6.0	5743.4	p5f2d ~ 1G1Ha 5.0	275 504.9
371.855		35	1.80E + 11	0.66	268 922.0	371.855	0.000	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I1Gb 4.0	271 756.6
372.550		39	3.78E + 11	-0.88	268 420.4	372.550	0.000	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F3Df 2.0	276 205.0
372.828		58	6.42E + 11	-0.82	268 220.2	372.828	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3H 4.0	276 531.3
373.070		40	4.91E + 11	0.73	268 046.2	373.070	0.000	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F3Ff 3.0	275 831.0
373.564		68	4.22E + 11	0.90	267 691.7	373.564	0.000	p6-f2_3F 2.0	5893.8	p5f2d ~ 1S3D 3.0	273 585.8
373.819		102	1.03E + 12	-0.94	267 509.1	373.814	0.005	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Gf2 5.0	273 256.0
374.261		36	8.80E + 11	0.90	267 193.2	374.261	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 1G1Ha 5.0	275 504.9
374.390		78	1.86E + 12	0.93	267 101.1	374.390	0.000	p6-f2_1I 6.0	260 88.1	p5f2d ~ 1I1Kb 7.0	293 189.0
374.658		91	9.85E + 11	-0.92	266 910.1	374.658	0.000	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F3Gd 4.0	274 695.0
374.930		105	1.06E + 12	0.89	26 6716.5	374.930	0.000	p6-f2_1G 4.0	122 69.7	p5f2d ~ 1G1G 4.0	278 986.5
375.151		36	1.64E + 11	0.87	266 559.3	375.151	0.000	p6-f2_3F 3.0	7784.8	p5f2d ~ 1I3Gb 3.0	274 344.0
375.451		119	1.32E + 12	0.93	266 346.3	375.451	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 3H3Ia 5.0	266 346.0
375.641D		174	1.57E + 12	0.93	266 211.6	375.641	0.000	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H3Ie 6.0	269 046.0
375.641D		174	1.78E + 12	-0.92	266 211.6	375.641	0.000	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Id 7.0	271 955.0
376.458		114	7.91E + 11	0.92	265 633.9	376.458	0.000	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I1Hb 5.0	268 468.0
377.058		68	1.59E + 12	-0.94	265 211.2	377.058	0.000	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3He 6.0	270 954.6
377.432		19	3.94E + 11	0.83	264 948.4	377.437	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H3Gf2 5.0	273 256.0
408.012		16	6.87E + 09	-0.03	245 090.8	408.011	0.001	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Gb 5.0	253 402.8
412.657	20	60	2.48E + 09	-0.03	242 332.0	412.658	-0.001	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F3Hb 6.0	245 165.8
412.734		45	1.67E + 09	-0.01	242 286.8	412.740	-0.005	p6-f2_3H 6.0	5743.4	p5f2d ~ 1G1K 7.0	248 026.8
413.770	9	42	1.16E + 09	-0.18	241 680.2	413.774	-0.004	p6-f2_3H 4.0	0.0	p5f2d ~ 3F3Gb 3.0	241 677.8
417.562		40	3.24E + 09	0.08	239 485.4	417.568	-0.006	p6-f2_3H 4.0	0.0	p5f2d ~ 3P3Fa2 3.0	239 482.1
420.851	98	96	1.43E + 10	-0.06	237 613.8	420.854	-0.003	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Kc 7.0	243 355.7
421.607		19	1.60E + 09	0.07	237 187.7	421.612	-0.005	p6-f2_3H 4.0	0.0	p5f2d ~ 1D3Ga 3.0	237 184.8
424.125	42	42	2.98E + 09	-0.03	235 779.6	424.117	0.008	p6-f2_3F 2.0	5893.8	p5f2d ~ 3F3Gb 3.0	241 677.8
427.543		22	2.11E + 09	0.03	233 894.6	427.546	-0.003	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F3Gb 3.0	241 677.8
427.680	27	62	3.28E + 09	-0.06	233 819.7	427.684	-0.004	p6-f2_3H 4.0	0.0	p5f2d ~ 3H3Ga 3.0	233 817.4
428.117bl		30	5.62E + 09	-0.09	233 581.0	428.117	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 1G3Ia 5.0	233 581.0
428.952	17	19	1.88E + 09	0.01	233 126.3	428.944	0.009	p6-f2_3H 5.0	2834.3	p5f2d ~ 3P5Fb 5.0	235 965.1
429.107	67	49	1.21E + 09	0.00	233 042.1	429.104	0.003	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Ib 7.0	238 787.0
430.296	11	4	3.45E + 08	0.01	232 398.2	430.291	0.005	p6-f2_3F 2.0	5893.8	p5f2d ~ 1G3Db 3.0	238 294.8
430.601	46	33	1.91E + 09	-0.04	232 233.6	430.601	0.001	p6-f2_3F 2.0	5893.8	p5f2d ~ 3F3Df 2.0	238 127.6
431.594	39	39	1.25E + 09	-0.04	231 699.2	431.598	-0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P3Fa2 3.0	239 482.1
432.356D	36	51	3.88E + 09	0.03	231 290.9	432.346	0.010	p6-f2_3H 4.0	0.0	p5f2d ~ 3H3Ha 4.0	231 296.1
432.356D	36	51	3.18E + 09	-0.04	231 290.9	432.356	0.000	p6-f2_3F 2.0	5893.8	p5f2d ~ 1D3Ga 3.0	237 184.8
432.389bl	62	50	1.65E + 09	-0.03	231 273.2	432.393	-0.004	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ga 5.0	234 105.4
432.448	10	30	8.12E + 08	0.01	231 241.7	432.450	-0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 3H1Ga 4.0	231 240.8
432.577		20	9.20E + 08	0.03	231 172.7	432.581	-0.004	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P3Fa2 3.0	239 482.1

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA s ⁻¹	CF	σ_{exp} (cm ⁻¹)	λ_{Ritz} (Å)	$\Delta\lambda$ (Å)	Lower level label	E _{low}	Upper level label	E _{up}
	PP	IP									
432.810		34	1.52E + 09	0.20	231 048.3	432.813	-0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 3P5Pb2 3.0	231 046.4
432.960	64	67	8.52E + 09	0.06	230 968.2	432.961	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 1I3Ib 5.0	230 967.9
433.130D	36	41	3.32E + 09	0.05	230 877.6	433.132	-0.002	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P5Fb 4.0	238 661.2
433.130D	36	41	3.16E + 09	0.06	230 877.6	433.130	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P3Fa 3.0	239 188.9
433.366	56	61	3.25E + 09	0.10	230 751.8	433.376	-0.009	p6-f2_3H 5.0	2834.3	p5f2d ~ 1G3Ia 5.0	233 581.0
433.820	30	29	4.08E + 08	0.01	230 510.4	433.821	-0.001	p6-f2_3F 3.0	7784.8	p5f2d ~ 1G3Db 3.0	238 294.8
434.131	58	53	2.45E + 09	-0.03	230 345.2	434.136	-0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F3Df 2.0	238 127.6
434.350bl	23	26	6.99E + 08	-0.01	230 229.1	434.364	-0.014	p6-f2_3H 6.0	5743.4	p5f2d ~ 3P5Fb 5.0	235 965.1
434.808	22	49	7.51E + 08	-0.03	229 986.6	434.814	-0.006	p6-f2_3F 4.0	8311.4	p5f2d ~ 1G3Db 3.0	238 294.8
436.840	168	87	3.63E + 10	-0.81	228 916.8	436.840	0.000	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3La 7.0	255 005.0
437.166	23	26	5.69E + 08	-0.02	228 746.1	437.183	-0.017	p6-f2_3H 4.0	0.0	p5f2d ~ 3P3Fc 4.0	228 737.2
437.401	26	20	1.53E + 09	0.02	228 623.2	437.400	0.001	p6-f2_3H 4.0	0.0	p5f2d ~ 3H5Fb 5.0	228 623.7
437.711	19	20	1.15E + 08	0.00	228 461.3	437.710	0.001	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H3Ha 4.0	231 296.1
437.812	77	54	8.62E + 09	-0.14	228 408.5	437.816	-0.004	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H1Ga 4.0	231 240.8
437.897	83	54	4.79E + 09	0.07	228 364.2	437.901	-0.004	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3Ga 5.0	234 105.4
438.228D	108	100	5.54E + 09	-0.25	228 191.7	438.232	-0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 3P5Pa 3.0	228 189.8
438.228D	108	100	1.01E + 10	-0.10	228 191.7	438.227	0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Ka 7.0	233 935.4
438.430	27	21	3.75E + 08	-0.03	228 086.6	438.431	-0.001	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P3Dc 2.0	233 979.7
438.742	48	36	5.89E + 09	0.12	227 924.4	438.744	-0.002	p6-f2_3F 2.0	5893.8	p5f2d ~ 3H3Ga 3.0	233 817.4
438.913	24	33	2.45E + 09	-0.15	227 835.6	438.909	0.004	p6-f2_3H 6.0	5743.4	p5f2d ~ 1G3Ia 5.0	233 581.0
439.265	8	20	2.68E + 09	0.04	227 653.0	439.264	0.001	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P5Fb 5.0	235 965.1
439.918bl	33	57	2.05E + 10	0.10	227 315.1	439.919	-0.001	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3Gb 5.0	253 402.8
440.129bl	24	20	3.19E + 09	-0.14	227 206.1	440.117	0.012	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P3Fa2 3.0	239 482.1
440.424	56	37	3.84E + 09	0.13	227 053.9	440.430	-0.006	p6-f2_3H 4.0	0.0	p5f2d ~ 1I3Ga3 3.0	227 051.0
440.685	30	35	1.79E + 09	-0.04	226 919.5	440.686	-0.001	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P3Fa 3.0	239 188.9
441.124	46	29	2.28E + 09	0.23	226 693.6	441.113	0.011	p6-f2_3H 5.0	2834.3	p5f2d ~ 1G3H 4.0	229 533.7
441.268	120	74	1.22E + 10	-0.08	226 619.7	441.271	-0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 3H3If 5.0	226 618.2
441.679		42	2.24E + 07	0.00	226 408.8	441.674	0.006	p6-f2_3H 4.0	0.0	p5f2d ~ 1I1Ha 5.0	226 411.4
441.714	44	46	1.16E + 10	0.13	226 390.8	441.713	0.001	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P5Fb 4.0	238 661.2
441.876	83	83	2.64E + 10	-0.28	226 307.83	441.876	0.000	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3La 7.0	252 396.0
441.986	43	53	1.58E + 09	0.05	226 251.5	441.967	0.019	p6-f2_3H 4.0	0.0	p5f2d ~ 1D3Gb 4.0	226 261.1
442.097	21	21	1.08E + 09	0.13	226 194.7	442.097	0.001	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P3Dc 2.0	233 979.7
442.216	49	41	2.88E + 08	0.10	226 133.8	442.214	0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 3P3De 3.0	226 134.9
442.424D	80	81	7.09E + 09	-0.17	226 027.5	442.414	0.010	p6-f2_3F 4.0	7784.8	p5f2d ~ 3H3Ga 3.0	233 817.4
442.424D	80	81	7.25E + 09	0.25	226 027.5	442.429	-0.005	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1G3Db 3.0	238 294.8
442.678	14	18	3.99E + 09	0.17	225 897.8	442.668	0.010	p6-f2_3H 5.0	2834.3	p5f2d ~ 3P3Fc 4.0	228 737.2
442.878D		21	1.53E + 09	-0.03	225 795.8	442.891	-0.012	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H5Fb 5.0	228 623.7
442.878D		21	1.10E + 09	0.01	225 795.8	442.882	-0.003	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Ga 5.0	234 105.4
443.066	68	41	1.29E + 09	-0.02	225 700.0	443.070	-0.004	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P3Fc 3.0	231 592.0
443.333	48	23	2.96E + 09	-0.03	225 564.1	443.332	0.000	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H5Ka 6.0	228 398.8
444.621	62	18	1.93E + 09	0.03	224 910.7	444.612	0.009	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1D3Ga 3.0	237 184.8

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA	CF	σ_{exp}	λ_{Ritz}	$\Delta\lambda$	Lower level	E_{low}	Upper level	E_{up}
	PP	IP	s ⁻¹		(cm-1)	(Å)	(Å)	label		label	
445.375	53	20	3.22E + 09	0.08	224 529.9	445.376	-0.001	p6-f2_3H 4.0	0.0	p5f2d ~ 1I3Ga 4.0	224 529.3
446.855	49	33	3.70E + 09	0.03	223 786.2	446.860	-0.004	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H3If 5.0	226 618.2
447.040bl	46	33	3.04E + 09	0.06	223 693.6	447.037	0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P5Fb 5.0	235 965.1
447.401	27	20	3.54E + 08	0.06	223 513.1	447.405	-0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 3H3Ha 4.0	231 296.1
447.514	60	46	2.51E + 09	-0.05	223 456.7	447.515	-0.001	p6-f2_3F 3.0	7784.8	p5f2d ~ 3H1Ga 4.0	231 240.8
447.560	117	76	1.46E + 10	-0.23	223 433.7	447.574	-0.014	p6-f2_3H 5.0	2834.3	p5f2d ~ 1D3Gb 4.0	226 261.1
447.875	52	51	2.21E + 09	-0.09	223 276.6	447.867	0.008	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P3Fc 3.0	231 592.0
447.920p	111	49	4.92E + 08	0.02	223 254.2	447.923	-0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 3H3Da 3.0	223 252.7
448.450	75	41	2.62E + 09	-0.07	222 990.3	448.461	-0.011	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H3Ha 4.0	231 296.1
448.572	50	29	2.68E + 09	-0.07	222 929.7	448.573	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H1Ga 4.0	231 240.8
448.671bl	146	87	1.93E + 10	0.24	222 880.5	448.671	0.000	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H5Fb 5.0	228 623.7
448.967bl	99	37	1.81E + 09	0.05	222 733.5	448.964	0.003	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P5Pb2 3.0	231 046.4
449.123D	75	26	5.63E + 09	0.04	222 656.2	449.125	-0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H5Ka 6.0	228 398.8
449.123D	75	26	2.48E + 09	-0.05	222 656.2	449.122	0.001	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Ib 5.0	230 967.9
449.506	33		1.59E + 09	-0.05	222 466.4	449.505	0.001	p6-f2_3H 4.0	0.0	p5f2d ~ 1I3Ha2 4.0	222 466.9
449.845	68		4.01E + 09	-0.10	222 298.8	449.851	-0.006	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P5Pa 3.0	228 189.8
450.322	41		1.08E + 09	0.02	222 063.3	450.326	-0.004	p6-f2_3H 4.0	0.0	p5f2d ~ 1D3Gb 5.0	222 061.2
450.580	115	65	1.55E + 10	-0.25	221 936.2	450.575	0.005	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1G1K 7.0	248 026.8
450.781	49	28	5.67E + 07	0.00	221 837.2	450.784	-0.003	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I3Ga 5.0	234 105.4
450.968	33	22	2.70E + 09	0.12	221 745.2	450.961	0.008	p6-f2_3F 3.0	7784.8	p5f2d ~ 1G3H 4.0	229 533.7
451.077	50		2.41E + 09	-0.11	221 691.6	451.070	0.007	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ga 4.0	224 529.3
451.217	44		2.11E + 08	0.00	221 622.9	451.208	0.009	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3H 6.0	224 461.6
451.371	88	41	1.12E + 09	-0.05	221 547.2	451.370	0.001	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H3Ga 3.0	233 817.4
451.640	100	84	2.62E + 08	-0.01	221 415.3	451.637	0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 3P5Fa 3.0	221 416.7
451.858	105	63	2.20E + 10	-0.49	221 308.5	451.852	0.006	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1G3Ia 5.0	233 581.0
452.015	144	122	8.67E + 09	0.24	221 231.6	452.034	-0.019	p6-f2_3F 4.0	8311.4	p5f2d ~ 1G3H 4.0	229 533.7
452.228	66	9	1.18E + 09	0.08	221 127.4	452.230	-0.002	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3F3Gb 3.0	241 677.8
452.406	61	26	1.65E + 10	-0.23	221 040.4	452.406	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 3H5H 3.0	221 040.4
452.524	90	41	1.32E + 10	0.14	220 982.8	452.527	-0.003	p6-f2_3F 4.0	8311.4	p5f2d ~ 1D1H 5.0	229 292.9
452.600	43	8	4.21E + 09	0.08	220 945.6	452.586	0.014	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P3Fc 4.0	228 737.2
452.744	73	16	5.27E + 09	0.20	220 875.4	452.745	-0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3If 5.0	226 618.2
452.881	77	23	4.51E + 09	0.04	220 808.6	452.878	0.003	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ha 6.0	223 644.5
452.991	30	9	4.74E + 08	-0.03	220 754.9	452.992	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 1I3Ha 4.0	220 754.5
453.176bl	84	34	2.40E + 09	0.06	220 664.8	453.169	0.007	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I1Ha 5.0	226 411.4
	89	155	4.60E + 10	-0.61	220 529.5	453.457	-0.004	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H5Ka 7.0	226 271.3
453.562	45	23	5.78E + 07	0.00	220 477.0	453.570	-0.009	p6-f2_3H 4.0	0.0	p5f2d ~ 3P5Fa2 5.0	220 472.9
453.659	28	13	6.99E + 08	0.01	220 429.9	453.667	-0.008	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P3Fc 4.0	228 737.2
453.914	24	28	6.13E + 08	0.01	220 306.1	453.901	0.012	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H5Fb 5.0	228 623.7
454.053D	84	72	6.70E + 09	0.32	220 238.6	454.061	-0.008	p6-f2_3H 5.0	2834.3	p5f2d ~ 1D3Fb 4.0	223 069.0
454.053D	84	72	2.27E + 09	0.06	220 238.6	454.048	0.005	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P3De 3.0	226 134.9
454.702	119	122	4.76E + 09	0.20	219 924.3	454.700	0.003	p6-f2_3H 6.0	5743.4	p5f2d ~ 1D3H 5.0	225 668.8

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA s ⁻¹	CF	σ_{exp} (cm-1)	λ_{Ritz} (Å)	$\Delta\lambda$ (Å)	Lower level label	E _{low}	Upper level label	E _{up}
	PP	IP									
454.791	72	47	4.27E + 09	0.11	219 881.2	454.789	0.002	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ha 5.0	222 716.4
455.194D	93	47	2.91E + 09	-0.05	219 686.6	455.196	-0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 3H5I 4.0	219 685.7
455.194D	93	47	6.10E + 09	0.19	219 686.6	455.202	-0.008	p6-f2_3F 2.0	5893.8	p5f2d ~ 3F5Hb 3.0	225 576.7
455.318	32		8.27E + 08	-0.04	219 626.7	455.306	0.013	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ha2 4.0	222 466.9
455.954	18	7	1.13E + 09	0.06	219 320.4	455.950	0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P3Fc 3.0	231 592.0
456.059	33	18	2.77E + 09	0.09	219 269.9	456.067	-0.007	p6-f2_3F 3.0	7784.8	p5f2d ~ 1I3Ga3 3.0	227 051.0
456.398	146	128	1.40E + 10	0.15	219 107.0	456.405	-0.007	p6-f2_3H 4.0	0.0	p5f2d ~ 1I3Ia 5.0	219 103.5
456.460	106	51	9.23E + 09	0.59	219 077.3	456.459	0.001	p6-f2_1I 6.0	26 088.1	p5f2d ~ 3F3Hb 6.0	245 165.8
456.575	58	60	1.08E + 09	0.03	219 022.1	456.566	0.009	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H3Ha 4.0	231 296.1
456.688	35	24	7.24E + 08	0.02	218 967.9	456.681	0.006	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H1Ga 4.0	231 240.8
456.765	74	58	2.57E + 08	-0.03	218 931.0	456.766	0.000	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3P3Fa2 3.0	239 482.1
457.171a	98	80	2.80E + 09	-0.07	218 736.5	457.165	0.006	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Ga3 3.0	227 051.0
457.212	233	206	2.67E + 10	0.26	218 716.9	457.209	0.002	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3H 6.0	224 461.6
457.380T	55	32	1.97E + 08	-0.01	218 636.6	457.376	0.005	p6-f2_3H 4.0	0.0	p5f2d ~ 3P5Fa 5.0	218 638.7
457.380T	55	32	1.27E + 09	-0.04	218 636.6	457.385	-0.004	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ia 6.0	221 468.6
457.380T	55	32	8.40E + 08	0.02	218 636.6	457.378	0.002	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3P3Fa 3.0	239 188.9
457.725	67	48	1.60E + 09	0.09	218 471.8	457.716	0.009	p6-f2_3F 3.0	7784.8	p5f2d ~ 1D3Gb 4.0	226 261.1
457.939	104	123	4.76E + 09	-0.12	218 369.7	457.936	0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 1D3Fb 4.0	218 371.0
458.099	29	16	7.18E + 08	-0.06	218 293.4	458.112	-0.012	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P5S2 2.0	224 181.2
458.498	64	34	3.39E + 09	-0.12	218 103.5	458.505	-0.008	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I1Ha 5.0	226 411.4
458.674	90	37	6.30E + 09	-0.07	218 019.8	458.672	0.002	p6-f2_3F 2.0	5893.8	p5f2d ~ 3F3Gd 3.0	223 914.6
458.817	29	14	1.12E + 09	0.03	217 951.8	458.822	-0.005	p6-f2_3F 4.0	8311.4	p5f2d ~ 1D3Gb 4.0	226 261.1
458.885D	124	78	1.47E + 10	0.21	217 919.5	458.892	-0.007	p6-f2_3H 4.0	0.0	p5f2d ~ 3P5Fa 4.0	217 916.4
458.885D	124	78	1.83E + 09	-0.23	217 919.5	458.884	0.001	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ha 4.0	220 754.5
458.921	143	47	1.06E + 10	-0.30	217 902.4	458.924	-0.003	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3Ha 6.0	223 644.5
459.087	63	15	5.39E + 09	-0.18	217 823.6	459.087	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P3De 3.0	226 134.9
459.157	17		7.95E + 08	0.03	217 790.4	459.154	0.003	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F5Hb 3.0	225 576.7
459.461	234	120	2.06E + 10	-0.36	217 646.3	459.477	-0.016	p6-f2_3H 5.0	2834.3	p5f2d ~ 3P5Fa2 5.0	220 472.9
459.606	16		1.92E + 09	-0.14	217 577.7	459.609	-0.003	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3F3Df 2.0	238 127.6
460.074D	85	32	3.29E + 09	-0.11	217 356.3	460.069	0.005	p6-f2_3F 2.0	5893.8	p5f2d ~ 3H3Da 3.0	223 252.7
460.074D	85	32	1.67E + 09	-0.03	217 356.3	460.072	0.002	p6-f2_3F 4.0	8311.4	p5f2d ~ 1D3H 5.0	225 668.8
460.106	120	50	5.52E + 09	0.12	217 341.2	460.105	0.001	p6-f2_3H 4.0	0.0	p5f2d ~ 3F3Hc 4.0	217 341.6
460.267D	50	19	7.72E + 08	0.05	217 265.2	460.267	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 3F5Hb 3.0	225 576.7
460.267D	50	19	7.42E + 09	0.25	217 265.2	460.262	0.005	p6-f2_1I 6.0	26 088.1	p5f2d ~ 3H3Kc 7.0	243 355.7
460.783	87	100	4.55E + 09	-0.04	217 021.9	460.780	0.003	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1D1H 5.0	229 292.9
460.898	15	15	2.52E + 09	0.08	216 967.7	460.887	0.011	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3Ha 5.0	222 716.4
461.089	32	27	7.86E + 08	-0.07	216 877.9	461.085	0.004	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P5S 2.0	222 773.5
461.152	49	23	1.62E + 09	-0.10	216 848.2	461.145	0.007	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H5I 4.0	219 685.7
461.366	83	41	5.60E + 09	0.20	216 747.7	461.373	-0.006	p6-f2_3F 3.0	7784.8	p5f2d ~ 1I3Ga 4.0	224 529.3
461.605	98	64	8.04E + 09	-0.31	216 635.4	461.609	-0.004	p6-f2_1D 2.0	20 551.4	p5f2d ~ 1D3Ga 3.0	237 184.8
461.893	95	60	7.64E + 09	0.16	216 500.4	461.895	-0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 3H5Kb 5.0	216 499.5

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA	CF	σ_{exp}	λ_{Ritz}	$\Delta\lambda$	Lower level	E _{low}	Upper level	E _{up}
	PP	IP	s ⁻¹		(cm-1)	(Å)	(Å)	label		label	
462.118	68	36	1.25E + 09	-0.12	216 394.9	462.115	0.003	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P5S2 2.0	224 181.2
462.199	71	54	1.53E + 09	-0.02	216 357.0	462.206	-0.007	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H5Fb 5.0	228 623.7
462.276	35	23	5.74E + 08	0.08	216 321.0	462.283	-0.007	p6-f2_3H 6.0	5743.4	p5f2d ~ 1D3Gb 5.0	222 061.2
462.387	55	30	3.78E + 09	0.07	216 269.1	462.387	0.000	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ia 5.0	219 103.5
463.138	32		1.95E + 09	-0.13	215 918.4	463.134	0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P5Pa 3.0	228 189.8
463.276	125	74	1.15E + 10	0.48	215 854.1	463.276	0.000	p6-f2_1I 6.0	26 088.1	p5f2d ~ 3H3Kc 6.0	241 942.1
463.315	36		2.86E + 09	0.07	215 835.9	463.331	-0.016	p6-f2_3H 4.0	0.0	p5f2d ~ 3F5G 5.0	215 828.5
463.375	88	36	4.48E + 09	0.07	215 807.9	463.383	-0.007	p6-f2_3H 5.0	2834.3	p5f2d ~ 3P5Fa 5.0	218 638.7
463.554a	61	19	4.14E + 09	-0.08	215 724.6	463.553	0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3Ia 6.0	221 468.6
463.814	39	22	3.19E + 09	0.26	215 603.7	463.815	-0.001	p6-f2_3F 4.0	8311.4	p5f2d ~ 3F3Gd 3.0	223 914.6
463.987D	81	77	2.81E + 09	-0.08	215 523.3	463.996	-0.009	p6-f2_3H 5.0	2834.3	p5f2d ~ 1I3Ka 6.0	218 353.2
463.987D	81	77	3.18E + 08	-0.02	215 523.3	463.988	0.000	p6-f2_3F 2.0	5893.8	p5f2d ~ 3P5Fa 3.0	221 416.7
464.102	46		2.38E + 08	-0.01	215 469.9	464.106	-0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 3H3Da 3.0	223 252.7
464.128	107	83	3.83E + 09	-0.16	215 457.8	464.130	-0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 3H5Ka 5.0	215 456.7
464.500	76	99	7.56E + 09	-0.24	215 285.3	464.502	-0.002	p6-f2_3F 3.0	7784.8	p5f2d ~ 1D3Fb 4.0	223 069.0
464.810	24		6.49E + 09	-0.15	215 141.7	464.799	0.011	p6-f2_3F 2.0	5893.8	p5f2d ~ 3H5H 3.0	221 040.4
464.944	26		7.01E + 08	0.04	215 079.7	464.939	0.005	p6-f2_3H 5.0	2834.3	p5f2d ~ 3P5Fa 4.0	217 916.4
465.504	51	35	1.62E + 09	-0.04	214 820.9	465.511	-0.008	p6-f2_3F 3.0	7784.8	p5f2d ~ 1I3Ga2 3.0	222 602.3
465.596	16		1.47E + 09	0.04	214 778.5	465.590	0.006	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I3Ga3 3.0	227 051.0
465.647	18		1.84E + 08	0.00	214 755.0	465.641	0.006	p6-f2_3F 4.0	8311.4	p5f2d ~ 1D3Fb 4.0	223 069.0
465.714	23		1.89E + 09	-0.05	214 724.1	465.702	0.012	p6-f2_3H 6.0	5743.4	p5f2d ~ 3P5Fa2 5.0	220 472.9
465.802	37	9	9.94E + 08	-0.02	214 683.5	465.805	-0.003	p6-f2_3F 3.0	7784.8	p5f2d ~ 1I3Ha2 4.0	222 466.9
466.074	97	68	1.47E + 09	0.04	214 558.2	466.069	0.005	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3Ka2 6.0	220 304.1
466.189	55	18	9.77E + 08	0.06	214 505.3	466.185	0.005	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F3Hc 4.0	217 341.6
466.401	23	33	1.03E + 09	-0.03	214 407.8	466.407	-0.006	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Ha 5.0	222 716.4
466.940	65	40	1.49E + 09	0.02	214 160.3	466.950	-0.010	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Ha2 4.0	222 466.9
466.976	27	26	8.45E + 08	0.03	214 143.8	466.981	-0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I1Ha 5.0	226 411.4
467.300	68	74	3.25E + 09	-0.12	213 995.3	467.309	-0.009	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1D3Gb 4.0	226 261.1
467.580	51	60	2.83E + 09	-0.15	213 867.2	467.584	-0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P3De 3.0	226 134.9
467.825	50	36	7.54E + 08	-0.01	213 755.1	467.829	-0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 1D3F 4.0	221 538.1
467.876	32		1.08E + 09	0.03	213 731.8	467.861	0.014	p6-f2_3H 4.0	0.0	p5f2d ~ 3H1Gb 4.0	213 738.5
468.023	48		2.19E + 09	-0.02	213 664.7	468.022	0.001	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H5Kb 5.0	216 499.5
468.101	27	31	5.71E + 07	0.00	213 629.1	468.095	0.006	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P5Fa 3.0	221 416.7
468.488	69	60	1.88E + 09	0.02	213 452.7	468.488	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 3F3Hd 5.0	213 453.0
468.602	23	29	1.40E + 09	0.02	213 400.7	468.606	-0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1D3H 5.0	225 668.8
468.921	58	38	1.44E + 09	-0.08	213 255.5	468.921	0.000	p6-f2_3F 3.0	7784.8	p5f2d ~ 3H5H 3.0	221 040.4
468.974	77	39	4.30E + 09	-0.09	213 231.4	468.984	-0.011	p6-f2_3F 4.0	8311.4	p5f2d ~ 1D3F 4.0	221 538.1
469.504bl	37	80	6.13E + 07	0.00	212 990.7	469.496	0.007	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F5G 5.0	215 828.5
469.552	77	98	7.25E + 08	0.02	212 969.0	469.550	0.002	p6-f2_3F 3.0	7784.8	p5f2d ~ 1I3Ha 4.0	220 754.5
469.711	39	27	8.05E + 08	0.01	212 896.9	469.714	-0.003	p6-f2_3H 6.0	5743.4	p5f2d ~ 3P5Fa 5.0	218 638.7
470.071	25	18	7.30E + 06	0.00	212 733.8	470.082	-0.010	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H5H 3.0	221 040.4

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA	CF	σ_{exp}	λ_{Ritz}	$\Delta\lambda$	Lower level	E_{low}	Upper level	E_{up}
	PP	IP	s ⁻¹		(cm ⁻¹)	(Å)	(Å)	label		label	
470.146	19		7.78E + 08	0.02	212 699.9	470.148	-0.003	p6-f2_II 6.0	26 088.1	p5f2d ~ 3H3Ib 7.0	238 787.0
470.326	21		2.28E + 09	-0.13	212 618.5	470.317	0.009	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H5Ka 5.0	215 456.7
470.350	29	38	7.32E + 08	-0.05	212 607.6	470.345	0.005	p6-f2_3H 6.0	5743.4	p5f2d ~ 1I3Ka 6.0	218 353.2
470.405	44	32	9.91E + 08	-0.03	212 582.8	470.402	0.003	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P5Pb 3.0	220 368.9
471.122	24		1.27E + 09	0.02	212 259.2	471.121	0.000	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I3Ga 4.0	224 529.3
471.183	6	13	9.39E + 08	0.06	212 231.8	471.176	0.006	p6-f2_3P 1.0	25 892.9	p5f2d ~ 3F3Df 2.0	238 127.6
471.353	21	18	4.26E + 08	0.01	212 155.2	471.339	0.014	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P5Fa2 5.0	220 472.9
471.567	72	49	2.67E + 09	-0.08	212 059.0	471.570	-0.003	p6-f2_3F 4.0	8311.4	p5f2d ~ 3P5Pb 3.0	220 368.9
471.916	25		5.32E + 08	0.02	211 902.1	471.919	-0.002	p6-f2_3F 3.0	7784.8	p5f2d ~ 3H5I 4.0	219 685.7
473.309	15	4	1.05E + 08	0.01	211 278.5	473.309	0.000	p6-f2_3H 4.0	0.0	p5f2d ~ 1G3Ga2 3.0	211 278.3
473.387	37	15	1.19E + 09	-0.03	211 243.7	473.379	0.008	p6-f2_3H 4.0	0.0	p5f2d ~ 3F3Gf 5.0	211 247.3
473.835bl	23	12	2.85E + 08	0.01	211 043.9	473.842	-0.008	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3P3Fc 3.0	231 592.0
473.969	55	18	8.49E + 08	-0.04	210 984.3	473.972	-0.003	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H3Da 3.0	223 252.7
474.111bl	34	33	3.85E + 08	-0.01	210 921.1	474.113	-0.002	p6-f2_3H 4.0	0.0	p5f2d ~ 3H5D 4.0	210 920.2
474.351	13		1.13E + 08	0.01	210 814.4	474.347	0.004	p6-f2_3P 2.0	27 478.7	p5f2d ~ 1G3Db 3.0	238 294.8
474.414bl	39		1.83E + 08	0.01	210 786.4	474.401	0.013	p6-f2_3F 4.0	8311.4	p5f2d ~ 1I3Ia 5.0	219 103.5
474.861D	46	35	1.10E + 09	0.01	210 587.9	474.859	0.002	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F3Ia 6.0	213 423.3
474.861D	46	35	4.11E + 08	-0.01	210 587.9	474.865	-0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 1D3Fb 4.0	218 371.0
474.953	31		2.60E + 08	0.01	210 547.2	474.956	-0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 3F3Hb 5.0	210 545.7
475.445	61	55	4.63E + 08	0.03	210 329.3	475.438	0.007	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I3Ga2 3.0	222 602.3
475.891bl	30		5.74E + 08	0.03	210 132.2	475.892	-0.002	p6-f2_3F 3.0	7784.8	p5f2d ~ 3P5Fa 4.0	217 916.4
475.984	26	42	5.12E + 08	0.03	210 091.1	475.998	-0.014	p6-f2_3H 6.0	5743.4	p5f2d ~ 3F5G 5.0	215 828.5
476.683	76	29	9.37E + 08	-0.03	209 783.0	476.664	0.019	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1D3Gb 5.0	222 061.2
477.870	29	22	5.66E + 08	-0.02	209 261.9	477.855	0.015	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1D3F 4.0	221 538.1
479.649	21		1.04E + 08	0.00	208 485.8	479.651	-0.002	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I3Ha 4.0	220 754.5
479.817	51	17	1.15E + 09	-0.01	208 412.8	479.816	0.001	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F3Gf 5.0	211 247.3
480.299	26		1.99E + 07	0.00	208 203.6	480.300	-0.001	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P5Fa2 5.0	220 472.9
480.445	28		5.30E + 08	0.01	208 140.4	480.437	0.008	p6-f2_3H 4.0	0.0	p5f2d ~ 3F3Gb 5.0	208 143.8
480.569D	28	15	3.16E + 08	0.02	208 086.7	480.571	-0.002	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H5D 4.0	210 920.2
480.569D	28	15	1.01E + 08	0.00	208 086.7	480.569	0.001	p6-f2_3P 1.0	25 892.9	p5f2d ~ 3P3Dc 2.0	233 979.7
480.740	33	7	1.39E + 09	-0.06	208 012.7	480.729	0.011	p6-f2_II 6.0	26 088.1	p5f2d ~ 1I3Ga 5.0	234 105.4
481.122	45		1.34E + 09	0.18	207 847.5	481.122	0.000	p6-f2_II 6.0	26 088.1	p5f2d ~ 3H3Ka 7.0	233 935.4
481.435D	67	22	2.59E + 09	0.06	207 712.4	481.437	-0.002	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F3Hb 5.0	210 545.7
481.435D	67	22	8.60E + 08	-0.04	207 712.3	481.435	0.000	p6-f2_3H 6.0	5743.4	p5f2d ~ 3F3Hd 5.0	213 453.0
481.509	37		5.82E + 08	0.01	207 680.4	481.510	-0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 3F3Ia 6.0	213 423.3
482.119bl	33		7.15E + 08	0.02	207 417.7	482.123	-0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H5I 4.0	219 685.7
482.741D	43		2.14E + 09	-0.02	207 150.4	482.746	-0.005	p6-f2_3H 4.0	0.0	p5f2d ~ 1G3Hb 5.0	207 148.2
482.741D	43		8.11E + 08	-0.01	207 150.4	482.753	-0.012	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H5Ka 5.0	215 456.7
483.474	35		2.76E + 08	0.01	206 836.4	483.480	-0.006	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1I3Ia 5.0	219 103.5
484.244	57	9	6.46E + 08	-0.02	206 507.5	484.240	0.003	p6-f2_3H 4.0	0.0	p5f2d ~ 1G3G 5.0	206 509.1
484.577	21		1.59E + 08	0.00	206 365.6	484.569	0.008	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3P5Fa 5.0	218 638.7

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA s ⁻¹	CF	σ_{exp} (cm-1)	λ_{Ritz} (Å)	$\Delta\lambda$ (Å)	Lower level label	E _{low}	Upper level label	E _{up}
	PP	IP									
485.529	34	8	3.76E + 08	-0.01	205 960.9	485.546	-0.017	p6-f2_3F 3.0	7784.8	p5f2d ~ 3H1Gb 4.0	213 738.5
486.050bl	18	11	2.01E + 08	-0.01	205 740.2	486.040	0.010	p6-f2_3H 4.0	0.0	p5f2d ~ 3F5Fb 4.0	205 744.4
486.795	25	9	1.32E + 08	0.00	205 425.3	486.791	0.004	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H1Gb 4.0	213 738.5
486.881	35	9	2.35E + 08	0.00	205 389.0	486.892	-0.011	p6-f2_3F 2.0	5893.8	p5f2d ~ 1G3Ga2 3.0	211 278.3
487.468	28		1.36E + 09	0.02	205 141.5	487.468	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 3F3Hd 5.0	213 453.0
487.629	10		4.85E + 08	0.01	205 073.9	487.634	-0.005	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3F3Hc 4.0	217 341.6
488.281bl	26		9.57E + 07	0.00	204 800.1	488.276	0.005	p6-f2_3H 6.0	5743.4	p5f2d ~ 3F3Hb 5.0	210 545.7
490.971	89	28	4.98E + 08	0.01	203 678.0	490.979	-0.008	p6-f2_3H 5.0	2834.3	p5f2d ~ 1G3G 5.0	206 509.1
491.084	11		2.21E + 08	0.03	203 631.1	491.087	-0.003	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3P5S2 2.0	224 181.2
491.169	23	16	1.94E + 08	0.00	203 595.9	491.168	0.001	p6-f2_3H 4.0	0.0	p5f2d ~ 3H3Gf 5.0	203 596.3
491.279	19	22	4.26E + 08	-0.01	203 550.3	491.259	0.020	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3F5G 5.0	215 828.5
491.422	8		1.16E + 08	-0.01	203 491.1	491.416	0.006	p6-f2_3F 3.0	7784.8	p5f2d ~ 1G3Ga2 3.0	211 278.3
491.730	31		4.31E + 08	0.03	203 363.6	491.731	-0.001	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3F3Gd 3.0	223 914.6
492.158	12		1.23E + 08	0.00	203 186.8	492.158	0.000	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H5Ka 5.0	215 456.7
492.695	42	12	4.77E + 08	-0.02	202 965.3	492.691	0.004	p6-f2_3F 4.0	8311.4	p5f2d ~ 1G3Ga2 3.0	211 278.3
492.769	36		2.72E + 08	0.00	202 934.8	492.767	0.003	p6-f2_3F 4.0	8311.4	p5f2d ~ 3F3Gf 5.0	211 247.3
492.830	67	22	2.18E + 09	-0.05	202 909.7	492.829	0.001	p6-f2_3H 5.0	2834.3	p5f2d ~ 3F5Fb 4.0	205 744.4
493.343	16		1.67E + 08	0.01	202 698.7	493.337	0.006	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3H3Da 3.0	223 252.7
493.571bl	23		1.40E + 08	0.00	202 605.1	493.562	0.009	p6-f2_3F 4.0	8311.4	p5f2d ~ 3H5D 4.0	210 920.2
494.061	60	38	6.28E + 08	0.02	202 404.2	494.070	-0.009	p6-f2_3H 6.0	5743.4	p5f2d ~ 3F3Gb 5.0	208 143.8
496.355	36		8.55E + 08	0.01	201 468.7	496.355	0.000	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H1Gb 4.0	213 738.5
496.512	64		3.53E + 08	0.02	201 405.0	496.512	0.000	p6-f2_3H 6.0	5743.4	p5f2d ~ 1G3Hb 5.0	207 148.2
497.838	28		9.50E + 07	-0.01	200 868.6	497.846	-0.008	p6-f2_1D 2.0	20 551.4	p5f2d ~ 3P5Fa 3.0	221 416.7
498.098	26	17	5.88E + 08	0.02	200 763.7	498.093	0.005	p6-f2_3H 6.0	5743.4	p5f2d ~ 1G3G 5.0	206 509.1
498.232	16	15	1.35E + 08	0.00	200 709.7	498.228	0.003	p6-f2_3P 2.0	27 478.7	p5f2d ~ 3P5Pa 3.0	228 189.8
498.685	10	10	2.00E + 08	0.02	200 527.4	498.678	0.007	p6-f2_1I 6.0	26 088.1	p5f2d ~ 3H3If 5.0	226 618.2
499.177	29	25	1.43E + 08	0.00	200 329.7	499.183	-0.006	p6-f2_3H 4.0	0.0	p5f2d ~ 3F5Fb 4.0	200 327.2
499.546	23		2.34E + 08	-0.01	200 181.8	499.542	0.003	p6-f2_1I 6.0	26 088.1	p5f2d ~ 3H5Ka 7.0	226 271.3
499.872	41		3.65E + 08	0.00	200 051.2	499.874	-0.002	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H3Id 6.0	202 884.9
500.421	43		3.52E + 08	-0.01	199 831.8	500.419	0.001	p6-f2_3F 4.0	8311.4	p5f2d ~ 3F3Gb 5.0	208 143.8
502.495	30		3.73E + 08	-0.02	199 007.0	502.491	0.004	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1G3Ga2 3.0	211 278.3
502.559	26		1.89E + 08	0.00	198 981.6	502.569	-0.011	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3F3Gf 5.0	211 247.3
503.093	26		2.62E + 08	-0.01	198 770.5	503.093	0.000	p6-f2_3H 5.0	2834.3	p5f2d ~ 3H3Ia 5.0	201 606.0
503.384D	39		3.37E + 08	-0.01	198 655.5	503.397	-0.013	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H5D 4.0	210 920.2
503.384D	39		1.58E + 09	0.01	198 655.5	503.382	0.002	p6-f2_3P 2.0	27 478.7	p5f2d ~ 3P3De 3.0	226 134.9
504.091	9		8.51E + 07	0.00	198 376.9	504.100	-0.009	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3H 6.0	224 461.6
504.547	22		1.98E + 08	-0.02	198 197.6	504.547	0.000	p6-f2_3F 4.0	8311.4	p5f2d ~ 1G3G 5.0	206 509.1
505.148	13		1.63E + 08	0.00	197 961.8	505.154	-0.006	p6-f2_3F 3.0	7784.8	p5f2d ~ 3F5Fb 4.0	205 744.4
505.425	54	29	1.25E + 09	-0.01	197 853.3	505.426	-0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Gf 5.0	203 596.3
507.251	55	41	5.01E + 08	0.01	197 141.1	507.250	0.001	p6-f2_3H 6.0	5743.4	p5f2d ~ 3H3Id 6.0	202 884.9
507.919	12		1.65E + 08	-0.02	196 881.8	507.922	-0.003	p6-f2_3P 1.0	25 892.9	p5f2d ~ 3P5S 2.0	222 773.5

Table 1. (Continued.)

λ (Å)	Int _{exp}		gA	CF	σ_{exp}	λ_{Ritz}	$\Delta\lambda$	Lower level	E _{low}	Upper level	E _{up}
	PP	IP	s ⁻¹		(cm ⁻¹)	(Å)	(Å)	label		label	
508.392	25		4.19E + 08	0.03	196 698.6	508.382	0.010	p6-f2_3P 2.0	27 478.7	p5f2d ~ 3P5S2 2.0	224 181.2
508.568	30	66	2.13E + 08	-0.03	196 630.5	508.574	-0.005	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3Ha 5.0	222 716.4
510.267	10	16	5.20E + 08	0.24	195 975.8	510.274	-0.007	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1D3Gb 5.0	222 061.2
513.634	27	20	1.92E + 08	0.00	194 691.2	513.632	0.002	p6-f2_3F 2.0	5893.8	p5f2d ~ 1G3Ga 3.0	200 585.8
514.828bl	8	34	1.09E + 08	-0.01	194 239.6	514.829	-0.001	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1G3G 5.0	206 509.1
514.887	17		3.95E + 08	0.03	194 217.4	514.891	-0.004	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3Ka2 6.0	220 304.1
515.326	11		1.07E + 08	0.01	194 051.9	515.321	0.004	p6-f2_3F 3.0	7784.8	p5f2d ~ 1G3F 4.0	201 838.5
516.056	33		2.29E + 08	-0.02	193 777.4	516.050	0.006	p6-f2_3F 2.0	5893.8	p5f2d ~ 3H3Db 1.0	199 673.6
516.720	15		7.06E + 07	0.00	193 528.4	516.724	-0.004	p6-f2_3F 4.0	8311.4	p5f2d ~ 1G3F 4.0	201 838.5
516.859	24		3.88E + 08	0.01	193 476.4	516.864	-0.005	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3F5Fb 4.0	205 744.4
518.668	24	15	2.09E + 08	0.00	192 801.6	518.670	-0.001	p6-f2_3F 3.0	7784.8	p5f2d ~ 1G3Ga 3.0	200 585.8
520.115	11		5.26E + 08	-0.02	192 265.2	520.115	0.000	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1I3Ka 6.0	218 353.2
520.797	21		9.02E + 07	0.00	192 013.4	520.791	0.006	p6-f2_3F 4.0	8311.4	p5f2d ~ 3F5Fb 4.0	200 327.2
527.512	7	9	7.37E + 07	0.00	189 569.1	527.513	-0.001	p6-f2_1G 4.0	12 269.7	p5f2d ~ 1G3F 4.0	201 838.5
528.159	24		1.07E + 08	0.00	189 336.8	528.159	0.000	p6-f2_1G 4.0	12 269.7	p5f2d ~ 3H3Ia 5.0	201 606.0
544.068	5		2.58E + 08	0.05	183 800.6	544.071	-0.002	p6-f2_3P 2.0	27 478.7	p5f2d ~ 1G3Ga2 3.0	211 278.3
552.305	23		1.52E + 08	0.04	181 059.4	552.303	0.002	p6-f2_1I 6.0	26 088.1	p5f2d ~ 1G3Hb 5.0	207 148.2
575.433	50		1.27E + 08	0.06	173 782.2	575.438	-0.005	p6-f2_3P 1.0	25 892.9	p5f2d ~ 3H3Db 1.0	199 673.6

p: line resolved on the plate but perturbed by a close line.

bl: line partially resolved in a blended emission peak with components of similar intensities.

a: asymmetrical line, when the components of the blend have different intensities.

D: doubly classified.

T: Triply classified.

Lower level label: read $5p^64f^2\ ^3H\ J=6$ for p6-f2_3H 6.0 and so on. Upper level label: read $5p^54f^25d(^1G)^1Ha\ J=5$ for p5f2d-1G1Ha 5.0 and so on.

Table 2. Odd-parity energy levels of the $5p^5 4f^2 5d$ configuration of Nd^{4+} . For each level are given: J, the total angular momentum; the experimental energy value and its uncertainty (in cm^{-1}); N, the number of transitions involved in its determination; $\Delta E = E_{\text{exp}} - E_{\text{th}}$; g_L , the calculated Landé factor and the leading LS component of the wavefunction (when two levels have the same leading component, a number 2 is added to the designation of the higher level).

J	E_{exp} (cm^{-1})	Unc. (cm^{-1})	N	E_{th} (cm^{-1})	ΔE (cm^{-1})	g_L	1st LS comp.	Perc.
1	199 673.6	1.7	2	199 636.6	37.0	0.501	(3H) 3Db	51%
4	200 327.2	2.1	2	200 548.4	-221.2	1.1	(3F) 5Fb	12%
3	200 585.8	1.4	2	200 518.5	67.3	0.959	(1G) 3Ga	15%
5	201 606.0	1.6	2	201 474.2	131.8	1.033	(3H) 3Ia	11%
4	201 838.5	1.3	3	201 460.9	377.6	1.17	(1G) 3F	24%
6	202 884.9	1.5	2	202 801.0	83.9	1.083	(3H) 3Id	13%
5	203 596.3	1.5	2	203 576.8	19.5	1.132	(3H) 3Gf	15%
4	205 744.4	1.6	4	205 602.2	142.2	1.153	(3F) 5Fb	15%
5	206 509.1	1.2	5	206 124.6	384.5	1.1	(1G) 3G	16%
5	207 148.2	1.3	3	207 438.1	-289.9	1.014	(1G) 3Hb	9%
5	208 143.8	2.0	3	208 204.8	-61.0	1.091	(3F) 3Gb	8%
5	210 545.7	1.6	3	210 238.8	306.9	1.089	(3F) 3Hb	9%
4	210 920.2	2.0	4	210 953.1	-32.9	1.145	(3H) 5D	11%
5	211 247.3	1.8	4	211 085.1	162.2	1.091	(3F) 3Gf	8%
3	211 278.3	1.2	6	211 467.9	-189.6	1.036	(1G) 3Ga2	18%
6	213 423.3	1.8	2	213 233.6	189.7	1.132	(3F) 3Ia	13%
5	213 453.0	2.8	3	213 230.4	222.6	1.098	(3F) 3Hd	9%
4	213 738.5	3.0	4	213 582.1	156.4	1.068	(3H) 1Gb	7%
5	215 456.7	1.8	4	215 343.8	112.9	1.08	(3H) 5Ka	7%
5	215 828.5	4.0	4	215 837.5	-9.0	1.048	(3F) 5G	14%
5	216 499.5	1.7	2	216 498.2	1.3	1.028	(3H) 5Kb	9%
4	217 341.6	1.7	3	217 834.8	-493.2	1.03	(3F) 3Hc	7%
4	217 916.4	1.8	3	218 075.7	-159.3	1.026	(3P) 5Fa	9%
6	218 353.2	1.6	3	218 087.7	265.5	1.016	(1I) 3Ka	13%
4	218 371.0	2.1	2	218 738.6	-367.6	1.033	(1D) 3Fb	13%
5	218 638.7	2.0	4	218 601.8	36.9	1.144	(3P) 5Fa	12%
5	219 103.5	2.2	4	219 381.8	-278.3	0.931	(1I) 3Ia	27%
4	219 685.7	1.6	4	219 783.2	-97.5	0.963	(3H) 5I	17%
6	220 304.1	2.0	2	220 482.5	-178.4	1.009	(1I) 3Ka	16%
3	220 368.9	1.8	2	220 089.3	279.6	1.207	(3P) 5Pb	11%
5	220 472.9	3.0	5	220 448.7	24.2	1.122	(3P) 5Fa2	15%
4	220 754.5	1.3	4	220 549.4	205.1	1.137	(1I) 3Ha	21%
3	221 040.4	2.1	4	221 244.6	-204.2	0.867	(3H) 5H	11%
3	221 416.7	1.9	4	221 271.5	145.2	1.078	(3P) 5Fa	18%
6	221 468.6	2.2	2	221 299.0	169.6	1.116	(1I) 3Ia	10%
4	221 538.1	3.0	3	221 706.5	-168.4	1.12	(1D) 3F	11%
5	222 061.2	3.0	4	222 239.8	-178.6	1.078	(1D) 3Gb	16%
4	222 466.9	2.3	4	222 409.8	57.1	1.064	(1I) 3Ha2	13%
3	222 602.3	3.0	2	222 780.7	-178.4	1.138	(1I) 3Ga2	11%
5	222 716.4	1.9	4	222 952.3	-235.9	1.006	(1I) 3Ha	18%
2	222 773.5	1.8	2	222 659.0	114.5	1.248	(3P) 5S	8%
4	223 069.0	2.0	3	223 425.8	-356.8	1.109	(1D) 3Fb	10%
3	223 252.7	1.4	5	223 287.1	-34.4	1.151	(3H) 3Da	13%
6	223 644.5	2.0	2	223 792.4	-147.9	1.078	(1I) 3Ha	10%
3	223 914.6	1.4	3	223 926.1	-11.5	1.032	(3F) 3Gd	7%
2	224 181.2	2.1	4	224 007.7	173.5	1.08	(3P) 5S2	9%
6	224 461.6	2.4	3	224 165.2	296.4	1.104	(1I) 3H	16%
4	224 529.3	1.6	4	224 892.1	-362.8	1.082	(1I) 3Ga	12%
3	225 576.7	2.1	3	225 655.1	-78.4	0.946	(3F) 5Hb	11%
5	225 668.8	1.7	3	225 261.6	407.2	1.077	(1D) 3H	9%
3	226 134.9	1.3	5	226 159.7	-24.8	1.219	(3P) 3De	14%
4	226 261.1	3.0	5	226 147.5	113.6	1.066	(1D) 3Gb	10%
7	226 271.3	1.9	2	226 316.3	-45.0	1.096	(3H) 5Ka	21%
5	226 411.4	1.9	4	226 646.3	-234.9	1.033	(1I) 1Ha	11%
5	226 618.2	1.6	4	226 408.9	209.3	0.936	(3H) 3If	27%
3	227 051.0	2.0	4	227 474.1	-423.1	1.065	(1I) 3Ga	8%

Table 2. (Continued.)

J	E_{exp} (cm ⁻¹)	Unc. (cm ⁻¹)	N	E_{th} (cm ⁻¹)	ΔE (cm ⁻¹)	g_L	1st LS comp.	Perc.
3	228 189.8	1.6	4	228 033.1	156.7	1.144	(3P) 5Pa	17%
6	228 398.8	2.1	2	228 375.6	23.2	1.049	(3H) 5Ka	7%
5	228 623.7	2.1	5	228 432.2	191.5	1.153	(3H) 5Fb	15%
4	228 737.2	3.0	4	228 582.6	154.6	1.127	(3P) 3Fc	11%
5	229 292.9	1.9	2	229 275.6	17.3	1.067	(1D) 1H	15%
4	229 533.7	4.0	3	229 497.9	35.8	1.032	(1G) 3H	11%
5	230 967.9	2.1	2	231 126.6	-158.7	0.958	(1I) 3Ib	16%
3	231 046.4	2.2	2	231 066.7	-20.3	1.264	(3P) 5Pb2	13%
4	231 240.8	1.4	5	231 269.0	-28.2	1.007	(3H) 1Ga	14%
4	231 296.1	2.1	5	231 749.9	-453.8	0.957	(3H) 3Ha	11%
3	231 592.0	1.9	4	231 776.3	-184.3	0.961	(3P) 3Fc	11%
5	233 581.0	2.0	4	233 665.2	-84.2	1.047	(1G) 3Ia	13%
3	233 817.4	1.7	4	233 969.6	-152.2	0.958	(3H) 3Ga	12%
7	233 935.4	1.9	2	233 927.6	7.8	1.06	(3H) 3Ka	21%
2	233 979.7	1.6	3	233 865.4	114.3	1.238	(3P) 3Dc	14%
5	234 105.4	1.9	5	234 115.9	-10.5	1.107	(1I) 3Ga	8%
5	235 965.1	3.0	4	236 080.5	-115.4	1.15	(3P) 5Fb	7%
3	237 184.8	2.1	4	237 367.7	-182.9	0.949	(1D) 3Ga	12%
2	238 127.6	1.6	4	238 063.1	64.5	1.009	(3F) 3Df	7%
3	238 294.8	1.5	5	238 705.8	-411.0	1.043	(1G) 3Db	7%
4	238 661.2	2.2	2	238 794.0	-132.8	1.108	(3P) 5Fb	9%
7	238 787.0	2.0	2	238 672.0	115.0	1.122	(3H) 3Ib	17%
3	239 188.9	1.9	3	239 515.6	-326.7	1.075	(3P) 3Fa	11%
3	239 482.1	1.9	5	239 330.5	151.6	1.05	(3P) 3Fa2	10%
3	241 677.8	1.9	4	241 613.1	64.7	0.98	(3F) 3Gb	9%
6	241 942.1	2.3	1	241 824.5	117.6	1.024	(3H) 3Kc	11%
7	243 355.7	3.0	2	243 270.9	84.8	1.092	(3H) 3Kc	21%
6	245 165.8	1.9	2	245 430.2	-264.4	1.052	(3F) 3Hb	11%
7	248 026.8	3.0	2	247 723.6	303.2	1.052	(1G) 1K	14%
7	252 396.0	3.0	1	252 339.5	56.5	1.034	(1I) 3La	12%
5	253 402.8	2.0	2	252 928.7	474.1	1.065	(1I) 3Gb	14%
7	255 005.0	3.0	1	254 967.4	37.6	1.003	(1I) 3La	26%
5	266 346.0	4.0	1	266 454.4	-108.4	0.852	(3H) 3Ia	25%
5	268 468.0	4.0	1	268 285.8	182.2	1.021	(1I) 1Hb	15%
6	269 046.0	5.0	1	269 084.8	-38.8	1.027	(3H) 3Ie	24%
6	270 954.6	3.5	1	271 191.1	-236.5	1.153	(3H) 3He	24%
4	271 756.6	3.6	1	271 860.2	-103.6	1.014	(1I) 1Gb	18%
7	271 955.0	5.0	1	271 933.4	21.6	1.132	(3H) 3Id	32%
5	273 256.0	4.0	2	273 230.1	25.9	1.18	(3H) 3Gf2	22%
3	273 585.8	3.6	1	273 113.2	472.6	0.982	(1S) 3D	12%
3	274 344.0	4.0	1	274 151.1	192.9	1.049	(1I) 3Gb	10%
4	274 695.0	4.0	1	274 845.4	-150.4	1.05	(3F) 3Gd	23%
5	275 504.9	3.5	2	275 553.1	-48.2	1.107	(1G) 1Ha	19%
3	275 831.0	4.0	1	275 476.4	354.6	1.095	(3F) 3Ff	20%
2	276 205.0	4.0	1	276 000.8	204.2	1.138	(3F) 3Df	24%
4	276 531.3	3.6	1	276 223.7	307.6	1.035	(1I) 3H	20%
4	278 986.5	3.6	1	279 248.2	-261.7	1.104	(1G) 1G	19%
7	293 189.0	4.0	1	293 317.6	-128.6	0.996	(1I) 1Kb	42%

Read (³H) ³Db for (3H) 3Db and so on.

3. Analysis and determination of energy levels

The analysis was supported by theoretical predictions by means of the Cowan's codes (RCN/RCN2/RCG/RCE) [18]. The starting point was given by a relativistic Hartree-Fock (HFR) calculation using the RCN code. Then *ab initio* values of electrostatic and spin-orbit radial integrals P_{HFR} , including CI integrals, were obtained as output of the RCN2 code. These *ab initio* values were then scaled by a proper scaling

factor (SF) before being injected as input for the diagonalization of the Hamiltonian by the RCG code. Initial SF values defined as $SF = P_{\text{fit}}/P_{\text{HFR}}$ can be estimated from neighboring spectra by regularities. In the present case, the previous parametric study of Nd V [10] already led to SF values for most of the parameters, in particular for $5p^6 4f5d$. For all CI Slater integrals, a SF of 0.64 was used. However, results on Ce IV [14] provided improved SF values for parameters involving the $5p^5$ subshell. The calculated (HFR)

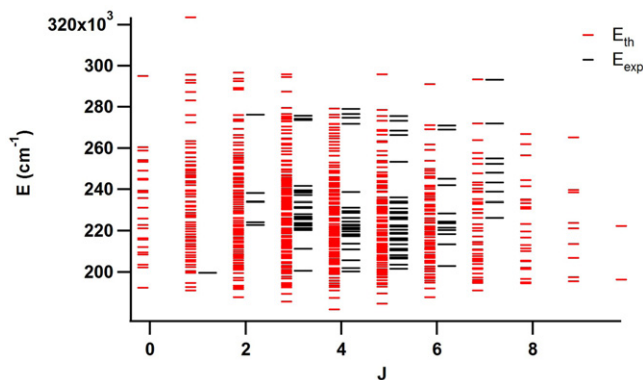


Figure 2. Energy levels of the $5p^5 4f^2 5d$ core-excited configuration. Red bars show the theoretical energies. The experimental energies are drawn with black long bars.

average energies of different configurations E_{av} were corrected by estimates from the experimental spectrum, in particular from the positions of the strongest emission arrays. In the present case, two transition arrays appeared at 380 and 450 Å, respectively.

Diagonalization of the Hamiltonian was performed with the same basis of configurations as in the previous work on Nd V [10]. On one hand, for the even parity the two known configurations $5p^6 4f^2$ and $5p^6 4f 6p$ were completed with three configurations with closed 5p sub-shell $5p^6 4f^2$, $5p^6 4f 6p$, $5p^6 (5d + 6s)^2$ and three core-excited configurations $5p^5 4f^3$, $5p^5 4f^2 6p$, $5p^5 4f 5d^2$, and on the other hand, the odd parity included the $5p^6 4f 5d$, $5p^6 4f 6s$, $5p^5 4f^2 5d$ and $5p^5 4f^2 6s$ configurations. Electric dipole transition probabilities were calculated. All these preliminary studies led to reliable predictions of unknown levels and transition probabilities.

Subsequently, when experimental level energies became available, the scaled radial integrals were used as adjustable parameters P_{fit} in a least-squares fit of energy levels by the RCE code. This fitting method was first applied by Racah in a two-electron spectrum Th III [19]. Using iteratively RCE and RCG during the progress of the analysis allowed continuous improvement of the theoretical predictions until the last least-squares fit that provided the final parameter values (Slater-Racah method).

To determine the energy levels of core-excited configurations, we started from the known levels of $5p^6 4f^2$ ground configuration and searched for the transitions to $5p^5 4f^2 5d$ and $5p^5 4f^2 6s$ in the range of 350–700 Å. The search for levels was essentially based on the Ritz combination principle and the comparisons between the observed spectral lines intensities and theoretical transition probabilities gA . The analysis was helped by using the IDEN code [20], which allows the visualization of a great amount of data for easier handling.

4. Results and discussion

The analysis of the spectrum led to the establishment of 104 levels of the $5p^5 4f^2 5d$ core-excited configuration by classifications of 304 spectral lines in the range of 370–575 Å.

Table 1 displays the classified line list and table 2, the energy levels determined. Most of these levels are determined through 2 to 5 transitions. Only the highest levels of the configuration are defined by one single but strong transition.

An optimization of the numerical values of level energies was carried out using the LOPT code [21] that minimizes the differences between the whole set of observed wave numbers of lines and those calculated by the Ritz principle from the experimental level energies. At the input of the code was the list of 304 wavelengths of classified lines. In the iterative least-squares procedure, the energies of the ground configuration levels had been fixed to their previous values [10], obtained by identifications of lines in longer wavelength region, thus allocated with smaller uncertainties on their wave numbers. The optimized level energies are presented in table 2, together with their quantum numbers J , their uncertainties and the number of lines involved in their determination. The final Ritz wavelengths of lines calculated with the optimized energy values are given in table 1, together with the labels and energies of the lower and upper levels of the transition. Figure 2 displays theoretical predicted positions and experimental positions of levels versus values of the total angular momentum J .

The structure of the transition array $5p^6 4f^2 - 5p^5 4f^2 5d$ is expected to be dominated by the $5p^6 \ ^1S - 5p^5 5d \ ^1P$ transition in the presence of the two $4f^2$ spectator electrons. The 1P term lies well above the other terms of the $5p^5 5d$ configuration, due to the large value of the Slater exchange integral $G^1(5p, 5d)$, and is rather pure. However, the small amount of mixture between the $J=1$ levels ($^1P - ^3P$ and $^1P - ^3D$) allows for the radiative decays from the lower levels of the $5p^5 4f^2 5d$ to $5p^6 4f^2$ in Nd V. This explains the transition array observed near 380 Å, due to $5p^5 4f^2 5d$ levels built on $5p^5 5d \ ^1P$, and the one near 450 Å, which is due to decays from the lower part of the $5p^5 4f^2 5d$.

As explained in section 2, the final loop RCE/RCG involved the set of experimental levels of table 2 and resulted in the final fitted energy parameter values. The calculations for the even parity configurations led to identical results as in [10]. Table 3 reports, for the odd parity configurations, the HFR and fitted energy parameters and their standard deviations in the least squares fit performed with 128 experimental levels, i.e. the newly determined 104 levels of $5p^5 4f^2 5d$ and the 24 previously determined [10] levels of $5p^6 4f 5d$ and $5p^6 4f 6s$. The corresponding mean deviation of the fit with 25 free parameters (see below) is 192 cm^{-1} . The corresponding diagonalization by RCG resulted in the calculated energies (E_{th}) and the Landé factors (g_L) given in table 2, as well as the level compositions of which the first LS components are given. The corresponding calculated gA values of transitions are given in table 1, as well as the corresponding cancellation factors (CF) defined by Cowan [18]. Although there are many |CF| less than or equal to 0.01, which means severe cancellation effects [22], they do not affect the reliability of the present determination of energy levels.

Calculations with the four odd configurations involve a matrix of maximum size 138×138 and 80 parameters, including off-diagonal Slater parameters R^k for first order CI

Table 3. Fitted parameters and Hartree-Fock integrals (in cm^{-1}) of odd-parity configurations of Nd^{4+} .

Param.	5p ⁶ 4f5d				5p ⁶ 4f6s				5p ⁵ 4f ² 5d				5p ⁵ 4f ² 6s		
	Fitted	St.dev.	HFR	SF	Fitted	St.dev.	HFR	SF	Fitted	St.dev.	HFR	SF	Adopted ^a	HFR	SF
Eav	136 706	260			196 690	156			227 202	25			277 784		
F ² (ff) r1									85 441	468	112 173	0.762	85 966	112 964	0.761
F ⁴ (ff) r1									60 447	331	70 884	0.853	60 856	71 427	0.852
F ⁶ (ff) r1									39 245	215	51 141	0.767	39 520	51 545	0.767
α									16	Fixed			16		
β									-432	Fixed			-432		
γ									1800	Fixed			1800		
ξ_f r2	1143	23	1150	0.994	1106	22	1157	0.976	1027	21	1075	0.955	1133	1083	1.046
ξ_{5p}									19 150	68	19 295	0.992	19 560	19 804	0.988
ξ_d r3	1515	51	1462	1.036					1353	46	1348	1.004			
F ² (fp)									39 574	Fixed	53 478	0.740	40 034	54 100	0.74
F ¹ (fd) r4	381	359							381	359					
F ² (fd) r5	26 592	422	34 558	0.769					24 272	385	33 870	0.717			
F ⁴ (fd) r6	18 174	682	17 210	1.056					20 197	758	17 002	1.188			
F ² (pd)									41 719	Fixed	54 820	0.761			
G ² (fp)									25 571	Fixed	26 246	0.974	25 689	26 375	0.974
G ⁴ (fp)									20 199	Fixed	20 824	0.970	20 378	21 008	0.970
G ¹ (fd) r6	11 874	211	13 653	0.870					10 626	189	14 314	0.742			
G ² (fd) r7	1145	563							1145	563					
G ³ (fd) r8	11 487	614	12 213	0.941					13 069	699	12 452	1.050			
G ⁴ (fd) r7	1145	563							1145	563					
G ⁵ (fd) r9	8881	513	9638	0.921					10 260	593	9736	1.054			
G ¹ (pd)									44 667	85	65 133	0.686			
G ³ (pd)									32 753	Fixed	40 940	0.800			
G ³ (fs)					2861	Fixed	3814	0.750					3929	3930	1.000
G ¹ (ps)													7106	7109	1.000
CI param.^b	Fitted	St.dev.	HFR	SF											
5p ⁶ 4f5d-5p ⁶ 4f6s															
R ² (fd.fs)	1796	96	2498	0.719											
R ³ (fd.sf)	2695	143	3748	0.719											
5p ⁶ 4f5d-5p ⁵ 4f ² 5d															
R ² (fp.ff)	-11 353	-604	-15 790	0.719											
R ⁴ (fp.ff)	-5682	-302	-7902	0.719											
R ² (pp.fp)	-26 231	-1396	-36 483	0.719											
R ² (pd.fd)	-19 721	-1049	-27 428	0.719											
R ⁴ (pd.fd)	-12 718	-677	-17 689	0.719											
R ¹ (pd.df)	-17 904	-953	-24 901	0.719											
R ³ (pd.df)	-12 893	-686	-17 932	0.719											
5p ⁶ 4f5d-5p ⁵ 4f ² 6s															

Table 3. (Continued.)

Param.	5p ⁶ 4f5d				5p ⁶ 4f6s				5p ⁵ 4f ² 5d				5p ⁵ 4f ² 6s		
	Fitted	St.dev.	HFR	SF	Fitted	St.dev.	HFR	SF	Fitted	St.dev.	HFR	SF	Adopted ^a	HFR	SF
R ² (pd.fs)	3412	181	4746	0.719											
R ¹ (pd.sf)	1669	89	2321	0.719											
5p ⁶ 4f6s-5p ⁵ 4f ² 5d															
R ² (pd.fd)	4351	231	6052	0.719											
R ³ (pd.df)	-1646	-88	-2289	0.719											
5p ⁶ 4f6s-5p ⁵ 4f ² 6s															
R ² (fp.ff)	-11 216	-597	-15 599	0.719											
R ⁴ (fp.ff)	-5592	-298	-7777	0.719											
R ² (pp.fp)	-26 303	-1400	-36 583	0.719											
5p ⁵ 4f ² 5d-5p ⁵ 4f ² 6s															
R ² (fd.fs)	1239	66	1723	0.719											
R ³ (fd.sf)	2517	134	3500	0.719											
R ² (pd.ps)	-9157	-487	-12 736	0.719											
R ¹ (pd.sp)	-3330	-177	-4631	0.719											

rn: for a given n, parameter values linked by a constant ratio in the least-squares fit.

a: fixed at chosen values for this unknown configuration.

b: all the CI Slater parameters are linked by their HFR ratios.

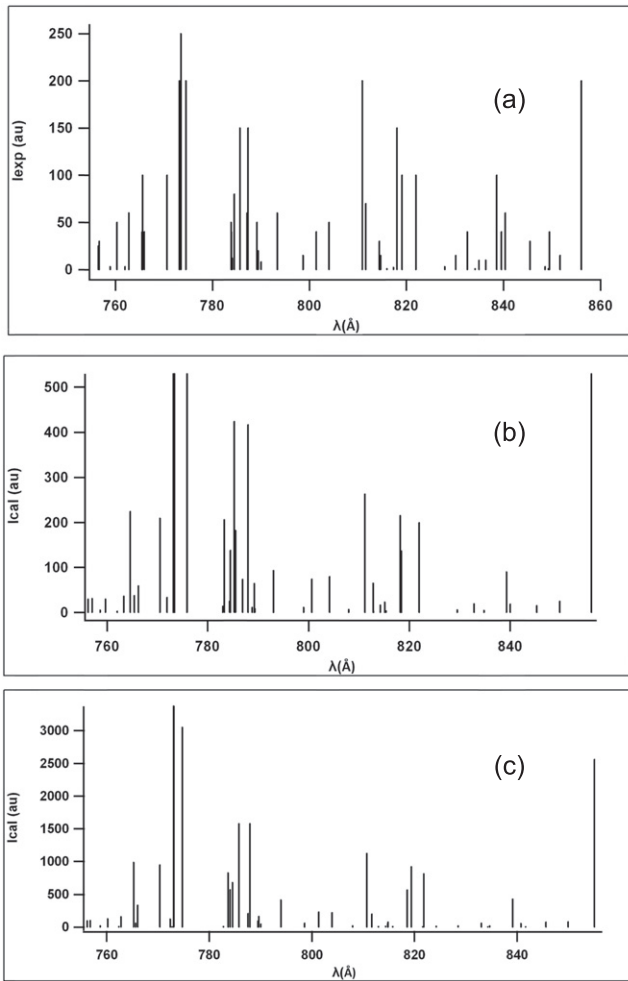


Figure 3. The $5p^6 4f^2 - 5p^6 4f 5d$ transitions in the wavelength region 755–860 Å: (a) intensities (in arbitrary units) of experimentally observed and identifies lines. (b) Intensities calculated including configuration interactions (CI) with $5p^5 4f^2 5d$ and $5p^5 4f^2 6s$. (c) Intensities calculated without CI. Both calculations with excitation temperature of 3.6 eV.

effects, effective parameters such as α , β , γ in $4f^2$ for second order perturbations from far configurations, and ‘Slater forbidden’ parameters for non-equivalent electrons [18]. However, in the present study, only 5 parameters were left as completely free in the least squares fit performed using the RCE code: the three configuration average energies E_{av} for $5p^6 4f 5d$, $5p^6 4f 6s$ and $5p^5 4f^2 5d$, the spin-orbit parameter ξ_{5p} of the sub-shell 5p, and the exchange integral $G^1(5p, 5d)$, the value of which fits the distance in energies between the two transition arrays at 380 Å and 450 Å. A number of electrostatic parameters were fixed with suitable scaling factors, chosen by comparison with earlier studies [9, 10]. In particular, for the unknown $5p^5 4f^2 5d$, the initial scaling factors were taken from the $5p^5 4f^3$ of Pr IV [23]. The electrostatic parameters common to both configurations $5p^6 4f 5d$ and $5p^5 4f^2 5d$ were varied simultaneously linked in the same ratio. In addition, all the CI parameters were forced to vary in the same ratio as their HFR values during the iteration process. They converged globally to 72% of their HFR values

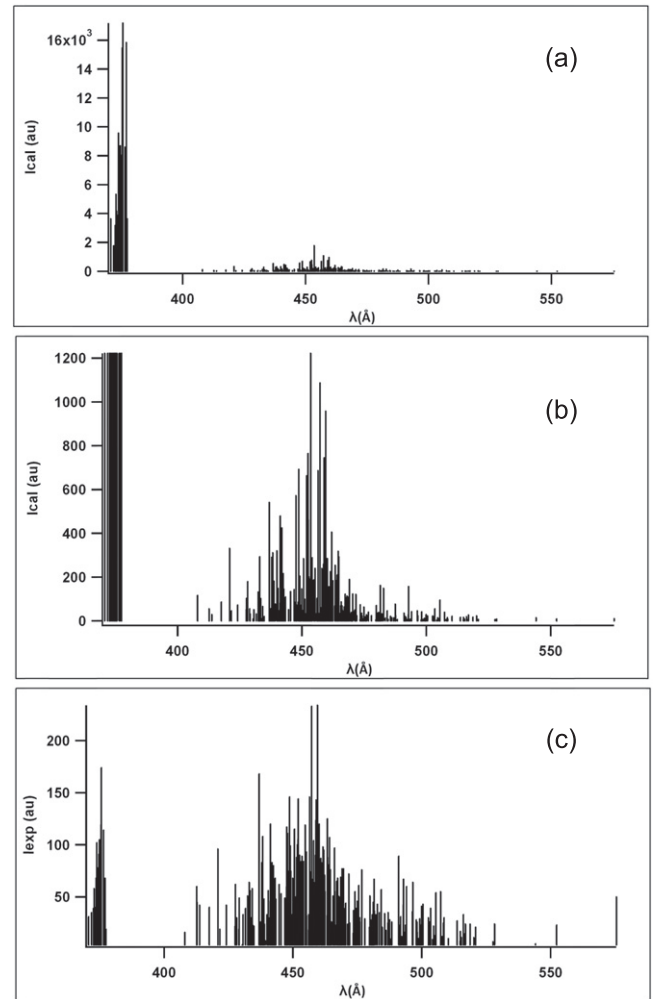


Figure 4. Comparison between the theoretical and experimental $5p^5 4f^2 5d - 5p^6 4f^2$ transition arrays. (a) Intensities calculated including CI with excitation temperature of 3.6 eV (b) idem, with expanded scale. (c) Experimentally observed and identified spectrum. The intensities of the short wavelength transition array are from image plates.

(SF = 0.72). The effective parameters were not given by the HFR calculations. Their initial values in the fit were chosen by comparisons with earlier studied cases. Finally the number of free parameters in the least-squares fit was 25.

Due to the presence of large number of new levels in the fitted system and constraints introduced, some differences between earlier [10] and our new values can be noticed for $5p^6 4f 5d$ and $5p^6 4f 6s$. One can notice that the present fit of CI parameters including experimental $5p^5 4f^2 5d$ levels led to a larger SF (0.72) than in reference [10] (SF = 0.64), which means a CI effect stronger than previously estimated. In the line list in [10], transition probabilities for the $5p^6 4f^2 - 5p^6 4f 5d$ transitions were compared in two approximations, with and without including the $5p^6 4f 5d - 5p^5 4f^2 5d$ interaction (columns 5 and 6 of table 3), showing a reduction of the gA values when including CI. The present fit strengthens this comparison, since our new gA values including stronger CI are, on average, 12% smaller than those obtained in [10] with CI included. Figure 3 displays for the wavelength region

750–850 Å a comparison between the experimentally identified spectrum [10] and two calculated spectra from the present work, one including CI, one without CI, assuming an excitation temperature of 3.6 eV.

In reference [10], it was predicted that a narrow transition array should appear around 380 Å corresponding to the strong 5p–5d transition in the $5p^64f^2-5p^54f^25d$ array. This prediction is confirmed by the results of the present work. Figure 4 displays for the wavelength region 375–550 Å a comparison between the experimentally identified spectrum and the calculated spectrum including CI, assuming an excitation temperature of 3.6 eV.

The calculated $5p^54f^25d$ configuration spreads from 18 1814 cm^{-1} (lowest level 5I_4) up to 32 3543 cm^{-1} (1P_1). Consequently, the $5p^54f^25d$ levels overlap the four levels of $5p^64f6s$ $^3F_{2,3,4}$ and 1F_3 at respectively 193 598.54, 194 029.49, 197 452.83 and 197 997.88 cm^{-1} , resulting in wavefunction mixings. In particular, the two $J = 3$ levels have wavefunctions with components belonging to $5p^54f^25d$. However, transitions from the $5p^64f6p$ levels to the $5p^54f^25d$ levels are not observed in our spectrograms.

5. Conclusion

We have extended the analysis of the Nd V spectrum by classification of 304 spectral lines in the wavelength region 370–575 Å leading to the determination of 104 previously unknown energy levels belonging to the core-excited configuration $5p^54f^25d$. At the end of the present work, the lowest part of the $5p^54f^25d$ configuration, mostly consisting of quintet states, stays unknown. Indeed, due to the insufficient breakdown of LS coupling in these quintet levels, their transitions to the ground configuration $4f^2$, comprising only singlets and triplets, have too small probabilities to be identified in the experimental line list. On the other hand, the search for the $5p^54f^3-5p^54f^25d$ system of transitions was considered by us as hopeless, given the small number of unclassified lines left on our plates in the predicted wavelength region near 1000 Å. Furthermore, none of the levels of the other core-excited configuration $5p^54f^26s$ could be localized in the present analysis. It is predicted to spread from 24 4952 to 34 4150 cm^{-1} by the parametric fit of the odd configurations, in which the same SF as for $5p^54f^25d$ were applied. Obviously, their possible knowledge would allow further improvement in theoretical gA values.

Acknowledgments

We are grateful to Dr N Spector for providing us the spectrogram earlier recorded at the NBS by himself and late Dr J Sugar, similarly to the ones already used in the previous Nd V

analysis [10]. The financial support of the French CNRS—PNPS national program is acknowledged. This work is part of the Plas@Par LabEx project managed by the ANR (ANR-11-IDEX-0004-02). DD and AM wish to acknowledge support from Université Mouloud Mammeri, Tizi-Ouzou, Algeria and from the project CNEPRU D00520110032, Algeria.

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