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Analysis of the free ion Nd^{3+} spectrum (Nd IV)

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Abstract

A recent breakthrough in the analysis of Nd IV resulted in the establishment of 37 energy levels of the ground configuration $4f^3$. We report here the completion to all 41 levels of this configuration. Wavelength measurements extended to 2800 Å and in higher excitation conditions lead to the classification of 1426 lines involving the excited configurations $4f^25d$, $4f^26p$, $4f^26s$. Owing to configuration mixing between $5p^64f^26p$ and the core-excited $5p^54f^4$, numerous $5p^64f^25d$–$5p^54f^4$ transitions, normally dipole-forbidden, are observed. Altogether 111 odd parity levels and 121 even parity ones have been established. Their parametric least-squares fits have rms deviations of 91 cm^{-1} and 37 cm^{-1}, respectively. The interaction $5p^64f^25d$–$5p^54f^35d$ has an impact on the $4f^3$–$4f^25d$ transition probabilities computed by means of the Cowan codes. Theoretical values of lifetimes are reported for all the even parity levels.

S This article has associated online supplementary data files

1. Introduction

Investigations on the spectroscopic properties of triply ionized lanthanides emitted by sparks have been resumed recently. After a 30-year period which followed the critical compilation of lanthanides energy levels by Martin *et al* [1], the first results in an unknown spectrum were obtained for Nd IV [2]. In that initial publication, we had recalled a number of reasons for studying spectra of a prohibitive complexity. Few ions have more applications than those of the trivalent lanthanides, especially Nd^{3+} for the laser at 1064 nm. The lowest 37 levels of the ground configuration $4f^3$ had been derived in [2] from $4f^3$–$4f^25d$ transitions. Their parametric interpretation had shown that improvements could be gained by including effective operators describing far configuration interactions (CI) [3]. The lowest configurations of Nd IV had been predicted by means of the codes by Cowan [4]. For deriving their energy levels with the diagonalization code RCG, the input Hartree–Fock radial integrals including relativistic corrections, treated as parameters (HFR parameters), were scaled according to earlier results on the neighbouring spectra [5–7]. The first steps in the previous parametric fitting process of Nd IV [2] by means of the RCE code led to better scaling factors for the radial integrals needed for the unknown configurations. This opened the way to the extended analysis reported below.

2. Experiment

The present work relies on the same experimental material as described in [2]. The neodymium spectrum emitted by a sliding spark [8, 9] was photographed on the 10.7 m normal incidence vacuum ultraviolet spectrographs at the National Institute of Standards and Technology (named NBS at the time of the exposures) and at the Paris-Meudon Observatory. The NBS instrument was equipped with a 1200 lines per mm ruled concave grating and provided a plate factor of 0.78 Å mm^{-1} in the first order. The Meudon spectrograph has a 3600 lines per mm holographic concave grating leading to a linear dispersion of 0.26 Å mm^{-1} on the plates. At NBS, the source operating conditions were varied to produce peak currents of 50, 200, 500 and 1200 A in order to discriminate lines from different ionic charges (Nd III to Nd V). Whereas the Nd IV lines interpreted as $4f^3$–$4f^25d$ transitions display equal intensities at peak currents 50 and 500 A, another class of lines in the range of 1200–1500 Å presents a steep current dependance, which varies from very weak (or absent) at 50 A to very strong at 1200 A. These lines are in the range of the predicted array from $4f^26p$ to $4f^25d$ in Nd IV. Around 2350 Å and 2650 Å two groups of lines have the same intensity behaviour and had been attributed in an early attempt of classification in Nd IV by Irwin [10] to the $4f^26p$–$4f^26s$ transitions.

In our initial study [2], for the wavelength measurements of the resonance transition array, the few sharper lines obtained at lower current had been preferred to those of richer spectra obtained at higher current. For the present extension of the level scheme, the high current tracks of the spectrograms were measured at Meudon on the same semi-automatic photoelectric comparator as in the previous work [2]. Wavelength standards for polynomial interpolation were taken from impurity lines of ionized low-Z elements (C, N, O, Al, Si) present in the Nd tracks [11] or from the neodymium wavelengths measured at weaker excitation. The estimated error is ±0.005 Å for single lines, but many lines are blended in complex emission peaks.

3. Determination of energy levels

In order to locate high energy levels, we started from the known $4f^25d$ levels and searched the 1200–1500 Å range for their combinations with $4f^26p$. The 6s–6p transitions lie in the region above 2200 Å. We found more odd parity levels than can be accounted for by the $4f^26p$ configuration, indicating the presence of another odd parity configuration. Our previous study [2] showed $5p^54f^4$ to be the first excited configuration in the odd parity. This configuration should be metastable in the absence of interaction with $4f^26p$, but the HFR Slater integrals $R^2(4f4f, 5p6p) = 7149$ cm^{-1} and $R^4(4f4f, 5p6p) = 6247$ cm^{-1} are large enough to produce configuration mixing and to permit transitions from $5p^54f^4$ to $5p^64f^25d$.

In order to support the search for levels by comparisons between the observed spectral line intensities and theoretical transition probabilities, we had to obtain realistic wavefunctions from an optimal set of radial parameters, by means of the diagonalization code RCG and least-squares fitting code RCE [4]. The iterative fitting process followed by RCE easily diverges if the theoretical levels do not match the ordering of the experimental levels from the first step of the fitting. Thus, in order to make the initial set of parameters for the

($5p^64f^3$, $5p^64f^26p$, $5p^54f^4$) group as close as possible to the final values, we estimated carefully the expected scaling factors $SF(P) = P_{\rm fit}/P_{\rm HFR}$ for the P parameters involved in the Hamiltonian operator. The $P_{\rm HFR}$ radial integrals were obtained by the Hartree–Fock code RCN that was run with relativistic corrections (HFR mode) without Breit energies, and with the correlation term set to a value of 1.0. Parameters for $4f^3$ had been determined in [2], and appropriate scaling factors for $4f^26p$ were derived from several earlier studies [5–7] and from the fit of $4f^25d$ levels in the opposite parity. Owing to the levels with evident $4f^26p$ character, an initial value of the average energy was easily estimated for this configuration.

The core-excited configurations in trivalent lanthanides had not yet been subject to a parametric study, so the assumed scaling factors for Nd IV $5p^54f^4$ had to be derived from $4f^3$ and $4f^25d$ in the same ion and from the $5p^54f$ configuration of Ce V [12] and La IV [13]. As for all the CI Slater integrals, the initial scaling factor used was 0.70. For an estimate of the average energy $E_{\rm av}(5p^54f^4)$ parameter, we compared the experimental and theoretical level schemes for $E_{\rm av}$ values incremented by steps of 1000 cm^{-1} around the HFR value. We found a unique set for which all experimental levels had an interpretation. From this set, the parametric fitting proceeded smoothly. A number of new levels with mixed characters ($5p^64f^26p$, $5p^54f^4$) confirmed the predicted energies and transition probabilities.

Our search for levels reached a point where the experimental evidence for new values became too uncertain. A number of missing levels are built on ^3P, ^1D, ^1S terms of $4f^2$ and have only a few transitions and these have low probabilities. The high odd configurations $4f^25f$, $4f5d^2$ and 4f5d6s are still missing whereas they are known in the isoelectronic spectrum of Pr III [14, 15]. In the 1200 A track of the Nd spark spectrum, an array of lines likely to fit the expected $4f^25f$–$4f^25d$ transitions is observed around 740 Å. However, its final interpretation is hampered by the overlap and mixing of $5p^64f^25f$ with $5p^54f^4$.

Altogether 111 odd parity and 121 even parity levels have been established. Their optimized values were calculated with the ELCALC code [16] which applies an iterative procedure to minimize the differences between the observed wave numbers and those calculated from level energies. As input to the code, 1314 classified lines were used with uncertainties on their wave numbers smoothly decreasing from 0.33 to 0.10 cm^{-1} between 1150 and 2800 Å. These optimized level values are listed, along with their uncertainties, in table 1 for the odd parity and in table 2 for the even parity. The customary unit (cm^{-1}) for level energies used here is related to the unit for energy (Joule) as $1\ cm^{-1} = 1.986\,445\,61\,(34) \times 10^{-23}$ J [17]. All levels are given a label of four characters, starting with the parity, respectively ‘e’ or ‘o’, followed by a single digit for the integer part of the J-value (highest observed J-value is 8.5). The last two digits indicate the numbering of the level within each J-value by increasing energies. In table 1, the terms for $4f^3$ are designated according to Martin *et al* [1]. The last columns of both tables are described in the following section.

A glimpse on the intricate level scheme of Nd IV odd parity levels is given in figure 1. The levels are represented by bars, the length of which is proportional to the amount of $4f^26p$ in the eigenfunction, starting from pure $5p^54f^4$ levels drawn with the shortest bars. For each J-value, the experimental levels are given on the right-hand side of the theoretical ones.

4. Theoretical interpretation

Locating the highest terms ^2G and ^2F of $4f^3$ is of particular interest for completing the study of the effects of far configurations. The application of orthogonal operators [3] to $4f^2$ in Pr IV [1] and in the newly analysed Nd V [18] and to the present $4f^3$ levels in Nd IV will be reported in a separate paper.

Table 1. Odd parity levels of Nd^{3+}. $\Delta E = E_{exp} - E_{th}$ and g_L is the calculated Landé factor. The sums of squared components for the main configurations are given in the last columns. The *LS* doublet terms of $4f^3$ are indexed as for Pr III in [1].

Conf.	Label	J	E_{exp} (unc.)	E_{th}	ΔE	g_L	First *LS*	comp. %	f^3 %	f^2p %	p^5f^4 %	fd^2 %
$4f^3$	o401	4.5	0.00 (13)	94	−94	0.732	^4I	96.8	99.84	0	0.13	0.04
$4f^3$	o501	5.5	1 897.11 (10)	1 985	−88	0.966	^4I	98.8	99.84	0	0.12	0.03
$4f^3$	o601	6.5	3 907.43 (10)	4 004	−97	1.107	^4I	99.4	99.85	0	0.12	0.03
$4f^3$	o701	7.5	5 988.51 (14)	6 105	−117	1.199	^4I	98.6	99.85	0	0.12	0.03
$4f^3$	o101	1.5	11 698.49 (8)	11 634	64	0.425	^4F	93.9	99.41	0	0.45	0.14
$4f^3$	o201	2.5	12 747.94 (7)	12 686	62	1.032	^4F	97.1	99.41	0	0.45	0.14
$4f^3$	o402	4.5	12 800.29 (6)	12 876	−76	1.006	$^2H2$	54.8	99.53	0.01	0.30	0.16
$4f^3$	o301	3.5	13 719.82 (6)	13 686	34	1.216	^4F	92.9	99.41	0	0.44	0.14
$4f^3$	o102	1.5	13 792.49 (8)	13 837	−45	1.961	^4S	94.2	99.58	0.01	0.26	0.15
$4f^3$	o403	4.5	14 994.87 (7)	14 986	9	1.234	^4F	75.0	99.45	0	0.40	0.14
$4f^3$	o502	5.5	16 161.53 (7)	16 224	−62	1.099	$^2H2$	79.9	99.57	0.01	0.27	0.16
$4f^3$	o202	2.5	17 707.17 (7)	17 596	111	0.575	^4G	97.8	99.26	0	0.56	0.18
$4f^3$	o302	3.5	17 655.11 (5)	17 623	32	0.939	$^2G2$	34.2	99.38	0.01	0.43	0.19
$4f^3$	o303	3.5	19 540.80 (6)	19 465	76	0.957	^4G	63.1	99.33	0	0.48	0.18
$4f^3$	o404	4.5	19 969.79 (5)	19 930	40	1.146	^4G	70.3	99.33	0	0.49	0.18
$4f^3$	o602	6.5	20 005.22 (8)	19 973	32	0.935	^2K	98.4	99.68	0	0.26	0.06
$4f^3$	o405	4.5	21 493.39 (6)	21 462	31	1.134	$^2G2$	37.1	99.40	0.01	0.41	0.18
$4f^3$	o103	1.5	21 700.90 (6)	21 745	−44	1.054	$^2D1$	47.8	99.36	0.02	0.37	0.24
$4f^3$	o702	7.5	22 043.77 (8)	22 014	29	1.063	^2K	94.4	99.69	0	0.26	0.05
$4f^3$	o503	5.5	22 047.39 (6)	22 032	15	1.261	^4G	92.4	99.29	0	0.53	0.17
$4f^3$	o001	0.5	23 788.93 (8)	23 779	10	0.624	^2P	93.2	99.41	0.03	0.31	0.25
$4f^3$	o203	2.5	24 333.10 (7)	24 369	−36	1.197	$^2D1$	97.1	99.36	0.02	0.37	0.25
$4f^3$	o104	1.5	26 761.19 (7)	26 792	−31	1.091	^2P	51.1	99.36	0.02	0.36	0.25
$4f^3$	o105	1.5	29 010.43 (6)	29 018	−7	1.139	^4D	81.3	98.89	0.01	0.81	0.29
$4f^3$	o204	2.5	29 190.91 (5)	29 155	36	1.329	^4D	78.8	98.85	0.01	0.84	0.30
$4f^3$	o002	0.5	29 540.41 (9)	29 595	−55	0.040	^4D	92.6	98.90	0.01	0.81	0.29
$4f^3$	o504	5.5	30 179.93 (6)	30 130	50	0.950	^2I	83.7	99.47	0.02	0.41	0.11
$4f^3$	o703	7.5	31 036.00 (11)	30 975	61	0.946	^2L	95.4	99.54	0	0.46	0
$4f^3$	o304	3.5	31 355.04 (6)	31 259	96	1.425	^4D	97.4	98.84	0	0.87	0.29
$4f^3$	o603	6.5	31 582.85 (6)	31 546	37	1.076	^2I	98.6	99.53	0.02	0.35	0.01
$4f^3$	o801	8.5	32 563.57 (12)	32 499	64	1.059	^2L	99.5	99.54	0	0.46	0
$4f^3$	o406	4.5	33 741.15 (6)	33 729	12	0.912	$^2H1$	86.2	91.11	0.01	0.71	0.17
$4f^3$	o106	1.5	34 275.21 (6)	34 281	−5	0.865	$^2D2$	79.2	98.98	0.02	0.66	0.33
$4f^3$	o505	5.5	35 136.61 (8)	35 143	−6	1.067	$^2H1$	67.9	99.18	0.01	0.65	0.16
$4f^3$	o205	2.5	35 213.92 (7)	35 200	14	1.169	$^2D2$	60.4	98.85	0.02	0.78	0.36
$4f^3$	o206	2.5	39 568.42 (6)	39 453	116	0.928	$^2F2$	44.6	98.80	0.01	0.73	0.46
$4f^3$	o305	3.5	41 012.70 (5)	40 909	104	1.145	$^2F2$	63.2	98.75	0.01	0.79	0.46
$4f^3$	o407	4.5	49 172.45 (10)	49 345	−172	1.110	$^2G1$	58.0	98.51	0.02	1.14	0.33
$4f^3$	o306	3.5	50 160.95 (6)	50 227	−66	0.892	$^2G1$	58.1	98.48	0.02	1.17	0.34
$4f^3$	o307	3.5	68 803.16 (10)	68 776	27	1.142	$^2F1$	63.9	97.89	0.01	1.29	0.81
$4f^3$	o207	2.5	69 932.59 (8)	70 093	−160	0.857	$^2F1$	57.4	97.90	0.01	1.30	0.79
$4f^26p$	o413	4.5	147 544.89 (7)	147 670	−125	0.804	$(^3H)^4I$	59.0	0	96.12	3.81	0.03
$4f^26p$	o313	3.5	147 943.06 (8)	147 872	71	0.772	$(^3H)^4H$	57.4	0	97.64	2.03	0.09
$5p^54f^4$	o314	3.5	147 964.38 (8)	147 940	25	1.114	$(^5F)^6G$	42.5	0	0.34	99.66	0
$4f^26p$	o415	4.5	150 560.55 (6)	150 478	82	1.032	$(^3H)^4H$	54.2	0	96.52	3.18	0.08

Table 1. (Continued.)

Conf.	Label	J	E_{exp} (unc.)	E_{th}	ΔE	g_L	First LS	comp. %	f^3 %	f^2p %	p^5f^4 %	fd^2 %
$4f^26p$	o512	5.5	150 607.32 (6)	150 614	−7	1.017	$(^3H)^4I$	49.8	0	95.64	4.25	0.07
$5p^54f^4$	o416	4.5	151 130.44 (6)	151 185	−55	1.024	$(^3H)^4H$	12.6	0.01	17.23	82.72	0.01
$5p^54f^4$	o417	4.5	152 592.92 (15)	152 504	90	0.870	$(^3H)^2H$	22.6	0.01	41.26	58.66	0.03
$5p^54f^4$	o513	5.5	152 592.63 (11)	152 464	128	1.093	$(^3H)^4H$	13.3	0	15.74	84.23	0.02
$4f^26p$	o214	2.5	152 710.30 (7)	152 722	−12	0.661	$(^3F)^4G$	41.4	0	84.57	15.22	0.09
$4f^26p$	o316	3.5	153 018.22 (7)	153 008	10	0.890	$(^3H)^4H$	30.5	0	84.18	15.47	0.07
$4f^26p$	o514	5.5	153 406.25 (7)	153 322	83	1.185	$(^3H)^4G$	41.9	0	95.56	4.13	0.07
$4f^26p$	o611	6.5	153 530.33 (7)	153 648	−117	1.162	$(^3H)^4H$	45.3	0	94.54	5.31	0.11
$5p^54f^4$	o418	4.5	153 628.29 (8)	153 455	173	0.780	$(^3K)^4I$	28.2	0.01	41.58	58.35	0.03
$5p^54f^4$	o610	6.5	153 724.25 (7)	153 816	−92	0.979	$(^3K)^2K$	17.3	0.01	0.89	99.11	0
$4f^26p$	o515	5.5	154 086.17 (6)	154 006	80	1.009	$(^3H)^2I$	30.8	0	73.30	26.55	0.12
$5p^54f^4$	o317	3.5	154 518.37 (5)	154 432	86	0.983	$(^3H)^4H$	5.5	0.02	13.43	86.50	0.01
$4f^26p$	o215	2.5	154 581.00 (8)	154 630	−49	0.653	$(^3H)^4G$	47.3	0.01	73.80	25.82	0.01
$4f^26p$	o318	3.5	154 812.25 (6)	154 856	−44	0.967	$(^3F)^4G$	33.3	0.01	78.48	21.36	0.07
$5p^54f^4$	o419	4.5	154 860.81 (7)	154 823	38	1.181	$(^3F)^4F$	11.5	0.02	18.65	81.27	0.02
$5p^54f^4$	o216	2.5	154 914.81 (5)	154 953	−39	0.917	$(^3F)^4D$	8.3	0.01	43.44	56.40	0.02
$5p^54f^4$	o517	5.5	155 363.07 (7)	155 485	−122	0.967	$(^3K)^4K$	19.0	0.01	19.63	80.34	0.01
$4f^26p$	o217	2.5	155 758.07 (7)	155 733	25	1.038	$(^3F)^4D$	22.8	0.01	71.04	28.71	0.04
$5p^54f^4$	o218	2.5	155 794.06 (7)	155 861	−67	1.074	$(^5G)^6G$	10.5	0	9.76	90.21	0.01
$4f^26p$	o518	5.5	155 870.45 (7)	155 995	−125	1.028	$(^3H)^2I$	47.3	0.01	79.99	19.78	0.16
$4f^26p$	o421	4.5	156 008.49 (5)	155 941	67	1.125	$(^3H)^4G$	21.7	0.01	62.24	37.57	0.05
$4f^26p$	o612	6.5	156 201.33 (8)	156 031	170	1.134	$(^3H)^4I$	43.1	0	66.19	33.74	0.05
$4f^26p$	o422	4.5	156 137.08 (5)	156 183	−46	1.093	$(^3F)^2G$	23.1	0.01	89.65	10.16	0.08
$4f^26p$	o320	3.5	156 272.69 (6)	156 291	−18	1.247	$(^3F)^4D$	43.4	0.01	96.07	3.53	0.11
$5p^54f^4$	o322	3.5		157 238		1.039	$(^3H)^4G$	14.5	0.01	36.20	63.62	0.01
$5p^54f^4$	o519	5.5	157 302.95 (8)	157 067	236	1.094	$(^3H)^4I$	7.1	0.02	16.20	83.75	0.01
$4f^26p$	o323	3.5	157 299.94 (6)	157 533	−233	1.041	$(^3H)^4G$	25.2	0.01	54.95	44.73	0.02
$5p^54f^4$	o522	5.5	158 032.30 (8)	158 264	−232	1.196	$(^3H)^4G$	21.6	0.01	49.01	50.83	0.04
$4f^26p$	o116	1.5	158 725.99 (10)	158 699	27	0.954	$(^3F)^4D$	43.0	0.05	73.33	26.33	0.07
$4f^26p$	o616	6.5	158 869.29 (9)	158 737	132	1.137	$(^3H)^2I$	50.3	0.02	79.86	19.92	0.18
$4f^26p$	o711	7.5	158 653.53 (11)	158 809	−156	1.197	$(^3H)^4I$	57.6	0	57.78	42.21	0.02
$4f^26p$	o221	2.5	159 266.54 (10)	159 262	4	1.053	$(^3F)^4F$	33.7	0.01	62.10	37.65	0.06
$4f^26p$	o326	3.5	159 585.51 (7)	159 605	−19	1.036	$(^3F)^2G$	33.7	0.01	90.82	8.88	0.12
$5p^54f^4$	o523	5.5	159 812.28 (10)	159 515	297	1.144	$(^3H)^2H$	15.2	0	31.69	68.21	0.03
$4f^26p$	o426	4.5	159 837.57 (6)	159 766	71	1.081	$(^3H)^2G$	44.6	0	95.60	3.92	0.11
$4f^26p$	o327	3.5	160 165.53 (7)	160 168	−3	1.113	$(^1G)^2G$	25.6	0.02	92.12	7.46	0.15
$4f^26p$	o427	4.5	160 420.64 (7)	160 324	96	1.115	$(^3F)^4G$	39.6	0.02	68.86	30.98	0.04
$4f^26p$	o119	1.5	160 657.90 (11)	160 713	−55	1.047	$(^3F)^4D$	28.1	0.04	57.45	42.28	0.07
$4f^26p$	o224	2.5	160 862.38 (7)	160 889	−27	1.117	$(^3F)^4D$	35.0	0.02	89.11	10.53	0.09
$4f^26p$	o429	4.5	161 225.30 (7)	161 199	26	1.176	$(^3F)^4F$	37.6	0.01	83.59	16.11	0.10
$4f^26p$	o329	3.5	161 496.05 (8)	161 384	111	1.137	$(^3F)^4F$	42.7	0.02	89.69	9.90	0.16
$4f^26p$	o526	5.5	161 574.84 (13)	161 594	−19	1.191	$(^3F)^4G$	51.3	0	76.97	22.87	0.07
$4f^26p$	o330	3.5	161 652.20 (10)	161 668	−16	1.091	$(^3F)^2F$	27.2	0.01	69.69	30.01	0.06
$4f^26p$	o226	2.5	161 901.82 (11)	161 884	18	1.046	$(^3F)^2F$	33.6	0.03	74.40	25.20	0.10
$4f^26p$	o432	4.5	162 034.11 (8)	162 251	−217	1.120	$(^3F)^2G$	34.7	0.03	85.50	13.99	0.27
$5p^54f^4$	o434	4.5	163 786.31 (10)	163 808	−22	1.025	$(^3I)^4I$	9.5	0.02	11.67	88.25	0.03
$5p^54f^4$	o436	4.5	164 957.81 (10)	164 851	107	1.173	$(^1G)^2G$	8.5	0.01	25.22	74.69	0.02

Table 1. (Continued.)

Conf.	Label	J	E_{exp} (unc.)	E_{th}	ΔE	g_L	First LS	comp. %	f^3 %	f^2p %	p^5f^4 %	fd^2 %
$5p^54f^4$	o530	5.5	165 158.58 (11)	164 952	207	1.164	$(^1G)^2H$	17.6	0.02	18.87	81.10	0.02
$4f^26p$	o232	2.5	165 183.48 (12)	165 274	−91	0.975	$(^1G)^2F$	54.9	0.02	93.03	6.55	0.10
$4f^26p$	o531	5.5	165 802.13 (11)	165 706	96	1.140	$(^1G)^2H$	49.4	0	78.31	21.56	0.10
$4f^26p$	o437	4.5	165 754.40 (13)	165 741	13	1.123	$(^1G)^2G$	23.9	0.01	52.82	47.00	0.05
$4f^26p$	o337	3.5	165 851.25 (9)	165 846	5	1.079	$(^1G)^2G$	22.6	0.04	60.68	38.94	0.13
$5p^54f^4$	o338	3.5	165 911.59 (12)	165 936	−25	1.176	$(^3F)^2F$	8.7	0.07	29.00	70.76	0.07
$5p^54f^4$	o439	4.5	166 908.81 (9)	167 072	−163	1.019	$(^3H)^4H$	9.2	0.05	10.30	89.62	0.01
$4f^26p$	o126	1.5		168 425		1.098	$(^1D)^2P$	32.3	0.01	56.81	42.91	0.10
$4f^26p$	o236	2.5		168 819		0.973	$(^1D)^2F$	35.7	0.02	56.87	42.81	0.11
$4f^26p$	o016	0.5		172 563		0.870	$(^1D)^2P$	31.0	0.01	69.31	30.24	0.29
$5p^54f^4$	o630	6.5	172 913.79 (8)	172 893	20	1.080	$(^1I)^2I$	18.8	0.01	29.18	70.72	0.09
$4f^26p$	o017	0.5		172 899		0.417	$(^3P)^4D$	47.3	0.03	84.34	15.21	0.22
$4f^26p$	o541	5.5	173 022.51 (7)	173 054	−32	0.990	$(^1I)^2I$	53.7	0	78.82	20.79	0.19
$4f^26p$	o018	0.5		173 594		1.701	$(^3P)^2S$	31.1	0.01	75.78	23.86	0.14
$4f^26p$	o350	3.5		173 641		1.145	$(^1D)^2F$	51.0	0.03	61.58	38.05	0.22
$5p^54f^4$	o631	6.5	173 949.03 (7)	173 814	135	1.060	$(^1I)^2I$	29.7	0.01	47.81	52.05	0.13
$4f^26p$	o133	1.5	174 355.70 (15)	174 321	34	1.289	$(^1D)^2P$	21.3	0.02	83.89	15.53	0.26
$4f^26p$	o134	1.5	174 586.13 (17)	174 580		1.301	$(^3P)^4D$	36.7	0.03	79.02	20.48	0.28
$4f^26p$	o244	2.5	174 803.78 (26)	174 839	−35	1.118	$(^1D)^2D$	17.5	0.04	53.83	45.82	0.10
$5p^54f^4$	o246	2.5	175 965.55 (17)	175 994	−29	1.162	$(^3P)^4D$	20.3	0.04	49.54	50.04	0.21
$4f^26p$	o635	6.5	178 165.59 (9)	178 263	−98	1.039	$(^1I)^2K$	30.6	0.01	50.52	49.30	0.17
$4f^26p$	o138	1.5		178 442		1.286	$(^3P)^4P$	35.1	0.01	86.80	12.40	0.44
$4f^26p$	o021	0.5		178 936		2.097	$(^3P)^4P$	53.1	0.01	87.15	12.30	0.22
$4f^26p$	o139	1.5		179 107		1.367	$(^3P)^2D$	31.6	0.03	82.95	16.33	0.35
$4f^26p$	o251	2.5	179 319.09 (26)	179 290	28	1.289	$(^3P)^2D$	27.9	0.02	63.29	36.15	0.34
$4f^26p$	o548	5.5	179 471.41 (9)	179 391	80	1.079	$(^1I)^2H$	40.6	0.01	53.11	46.35	0.12
$4f^26p$	o359	3.5	179 964.22 (14)	179 972	−8	1.280	$(^3P)^4D$	54.7	0.03	61.91	37.60	0.32
$4f^26p$	o728	7.5	180 284.96 (13)	180 323	−39	1.063	$(^1I)^2K$	81.2	0.01	81.50	18.23	0.26
$4f^26p$	o023	0.5		181 169		0.513	$(^3P)^2P$	39.0	0.07	55.67	43.63	0.34
$5p^54f^4$	o255	2.5	181 548.22 (13)	181 574	−26	1.098	$(^3P)^4P$	17.8	0.02	23.79	76.02	0.04

For the excited configurations of Nd IV with f-electrons and several open subshells, elaborate parametrizations based on the methods of group theory are not available for describing all the second-order CI effects. We used the possibilities of the Cowan codes [4], i.e. an extension of the basis of configurations for close level mixings and some of the effective parameters for interactions with far configurations. In the final parametric study of the odd parity, the three unknown configurations $5p^64f5d^2$, $5p^64f5d6s$ and $5p^64f6s^2$ were added to $5p^64f^3$+$5p^64f^26p$+$5p^54f^4$ discussed above. Indeed, the 4f6p–$5d^2$, 4f6p–5d6s and $4f^2-5d^2$ interactions have strong effects in the third spectra, Ce III [5] and Pr III, according to unpublished calculations by the first author. The sums of squared amplitudes pertaining to the main configurations are given in the last columns of table 1 and the fitted radial parameters are reported in table 3. Starting from the average values found in other lanthanides, the α, β, γ parameters for $4f^2$ and $4f^4$ were varied in a constant ratio. All CI Slater parameters were reduced to a single one by means of holding fixed the ratios of their HFR values. The small standard error of this single CI parameter corresponds to a scaling factor 0.96 ± 0.05. In $5p^54f^4$, the ratio F^4(f,f)/F^6(f,f) was held constant through the iterations.

Table 2. Even parity levels of Nd^{3+}. $\Delta E = E_{\rm exp} - E_{\rm th}$ and g_L is the calculated Landé factor. The sums of squared components for the three configurations are given in %. The theoretical lifetimes τ are given in the last column.

Conf.	Label	J	$E_{\rm exp}$ (unc.)	$E_{\rm th}$	ΔE	g_L	First LS	comp. %	f^2d %	f^2s %	p^5f^3d %	τ (ns)
$4f^25d$	e401	4.5	70 817.12 (9)	70 858	−41	0.832	$(^3H)^2H$	45.8	99.32	0	0.68	14.5
$4f^25d$	e501	5.5	71 744.57 (11)	71 772	−28	0.818	$(^3H)^4K$	75.1	99.54	0	0.46	116
$4f^25d$	e402	4.5	73 366.17 (8)	73 339	27	0.826	$(^3H)^4I$	50.5	99.36	0	0.64	16.9
$4f^25d$	e502	5.5	73 556.74 (8)	73 607	−50	1.019	$(^3H)^4I$	42.2	99.37	0	0.63	16.6
$4f^25d$	e201	2.5	73 616.22 (8)	73 683	−67	0.669	$(^3H)^4G$	46.4	99.34	0	0.66	29.9
$4f^25d$	e301	3.5	74 363.99 (10)	74 349	15	0.707	$(^3H)^4H$	83.3	99.12	0	0.88	6.9
$4f^25d$	e503	5.5	74 571.83 (7)	74 571	1	0.987	$(^3H)^4I$	52.7	99.39	0	0.61	17.0
$4f^25d$	e601	6.5	74 673.95 (15)	74 670	3	0.971	$(^3H)^4K$	93.6	99.52	0	0.48	133
$4f^25d$	e302	3.5	75 666.91 (7)	75 705	−38	0.976	$(^3H)^4G$	59.9	99.36	0	0.64	21.2
$4f^25d$	e403	4.5	76 411.72 (11)	76 406	6	0.992	$(^3H)^4H$	85.6	99.12	0	0.88	6.7
$4f^25d$	e602	6.5	76 471.40 (10)	76 483	−12	1.105	$(^3H)^4I$	96.9	99.30	0	0.70	10.8
$4f^25d$	e701	7.5	77 539.71 (21)	77 517	22	1.091	$(^3H)^4K$	99.1	99.51	0	0.49	134
$4f^25d$	e202	2.5	77 598.12 (7)	77 583	15	0.830	$(^3H)^2F$	29.9	99.12	0	0.87	21.2
$4f^25d$	e404	4.5	77 809.61 (6)	77 822	−13	1.139	$(^3H)^4G$	60.8	99.36	0	0.64	20.1
$4f^25d$	e303	3.5	77 833.03 (15)	77 851	−19	0.683	$(^3F)^4H$	91.3	99.21	0	0.79	8.6
$4f^25d$	e504	5.5	77 912.50 (6)	77 914	−1	1.011	$(^3H)^2I$	39.7	99.45	0	0.55	21.4
$4f^25d$	e505	5.5	78 702.59 (8)	78 692	10	1.091	$(^3H)^4H$	78.2	99.14	0	0.86	6.7
$4f^25d$	e702	7.5	78 864.24 (14)	78 873	−9	1.195	$(^3H)^4I$	95.4	99.30	0	0.70	10.7
$4f^25d$	e001	0.5	79 024.15 (12)	78 976	48	0.771	$(^3F)^2P$	55.6	99.07	0	0.92	12.7
$4f^25d$	e603	6.5	79 189.02 (9)	79 162	27	1.132	$(^3H)^2I$	45.4	99.42	0	0.58	15.6
$4f^25d$	e304	3.5	79 307.06 (6)	79 282	25	1.109	$(^3H)^2F$	28.9	99.04	0	0.96	15.1
$4f^25d$	e101	1.5	79 339.01 (9)	79 366	−27	0.424	$(^3H)^4F$	69.6	98.97	0	1.03	10.1
$4f^25d$	e405	4.5	79 694.96 (12)	79 713	−19	0.973	$(^3F)^4H$	91.5	99.22	0	0.77	9.04
$4f^25d$	e506	5.5	80 080.41 (8)	80 086	−6	1.234	$(^3H)^4G$	52.8	99.37	0	0.62	23.7
$4f^25d$	e203	2.5	80 128.30 (7)	80 113	15	0.872	$(^3H)^4F$	33.2	99.05	0	0.94	13.8
$4f^25d$	e801	8.5	80 431.49 (24)	80 389	42	1.177	$(^3H)^4K$	99.3	99.51	0	0.49	134
$4f^25d$	e102	1.5	80 663.34 (8)	80 647	16	1.451	$(^3F)^4P$	55.2	99.25	0	0.75	13.7
$4f^25d$	e204	2.5	81 013.13 (8)	81 019	−6	0.907	$(^3F)^4G$	39.0	99.13	0	0.87	15.2
$4f^25d$	e406	4.5	81 155.44 (7)	81 216	−61	1.089	$(^1G)^2H$	24.4	99.19	0	0.80	13.5
$4f^25d$	e604	6.5	81 303.91 (9)	81 293	11	1.174	$(^3H)^4H$	60.2	99.15	0	0.85	6.7
$4f^25d$	e305	3.5	81 375.35 (7)	81 400	−25	1.057	$(^3F)^2F$	33.3	99.25	0	0.75	22.3
$4f^25d$	e205	2.5	81 422.92 (7)	81 437	−14	1.223	$(^3F)^4P$	39.9	99.16	0	0.85	14.2
$4f^25d$	e002	0.5	81 502.48 (10)	81 440	62	2.206	$(^3F)^4P$	77.7	99.22	0	0.78	12.1
$4f^25d$	e507	5.5	81 691.09 (9)	81 698	−7	1.122	$(^3F)^4H$	88.2	99.24	0	0.76	9.77
$4f^25d$	e306	3.5	81 832.25 (7)	81 819	13	1.029	$(^3F)^4G$	51.8	99.07	0	0.93	15.9
$4f^25d$	e103	1.5	81 950.73 (10)	81 925	26	1.005	$(^3F)^4D$	42.5	99.06	0	0.94	11.0
$4f^25d$	e307	3.5	82 363.72 (9)	82 377	−14	1.054	$(^3F)^4F$	22.5	99.06	0	0.94	10.9
$4f^25d$	e407	4.5	82 669.72 (7)	82 658	11	1.192	$(^3H)^4F$	47.3	99.08	0	0.91	12.8
$4f^25d$	e104	1.5	83 032.16 (8)	83 007	25	1.010	$(^3F)^4D$	26.0	99.05	0	0.95	9.7
$4f^25d$	e605	6.5	83 309.16 (8)	83 327	−18	1.006	$(^3H)^2K$	63.6	99.17	0	0.83	12.8
$4f^25d$	e206	2.5	83 588.99 (8)	83 544	45	1.307	$(^3F)^4D$	78.2	98.96	0	1.04	8.9
$4f^25d$	e308	3.5	83 768.34 (8)	83 834	−66	1.089	$(^1G)^2F$	18.6	99.12	0	0.88	12.0
$4f^25d$	e508	5.5	83 903.04 (9)	83 905	−3	1.169	$(^1G)^2H$	29.4	99.08	0.01	0.91	16.7
$4f^25d$	e207	2.5	83 897.98 (6)	83 909	−11	1.018	$(^3F)^4F$	38.5	99.10	0	0.89	12.2
$4f^25d$	e606	6.5	84 092.98 (10)	84 101	−8	1.150	$(^3F)^4H$	69.8	99.25	0	0.75	12.0

Table 2. (Continued.)

Conf.	Label	J	E_{exp} (unc.)	E_{th}	ΔE	g_L	First LS	comp. %	f^2d %	f^2s %	p^5f^3d %	τ (ns)
$4f^25d$	e003	0.5	84 266.98 (10)	84 184	82	0.361	$(^3F)^4D$	58.5	99.00	0	1.00	9.72
$4f^25d$	e408	4.5	84 408.39 (7)	84 408	0	1.114	$(^3F)^4G$	51.2	99.13	0	0.86	18.3
$4f^25d$	e309	3.5	84 672.74 (8)	84 666	6	1.268	$(^3F)^4D$	60.9	98.96	0	1.04	8.93
$4f^25d$	e105	1.5	84 698.79 (7)	84 691	7	1.115	$(^3F)^2P$	34.3	99.08	0	0.91	12.3
$4f^25d$	e106	1.5	84 775.85 (8)	84 760	16	0.817	$(^3F)^4F$	18.6	99.06	0	0.94	12.7
$4f^25d$	e208	2.5	84 855.30 (7)	84 872	−17	1.164	$(^3F)^2D$	16.6	99.07	0	0.93	11.7
$4f^25d$	e409	4.5	85 352.26 (7)	85 338	13	1.147	$(^3F)^4F$	23.1	99.05	0	0.95	10.7
$4f^25d$	e410	4.5	85 716.11 (8)	85 745	−30	1.161	$(^3H)^2G$	37.4	99.12	0	0.87	13.8
$4f^25d$	e310	3.5	86 067.88 (7)	86 098	−30	1.085	$(^3F)^4F$	42.1	98.99	0	1.01	9.12
$4f^25d$	e703	7.5	86 678.25 (9)	86 656	21	1.071	$(^3H)^2K$	86.3	99.15	0	0.85	13.5
$4f^25d$	e509	5.5	87 072.95 (8)	87 020	53	1.068	$(^1G)^2I$	37.2	99.06	0	0.93	8.96
$4f^25d$	e209	2.5	87 114.19 (6)	87 092	22	1.107	$(^1G)^2D$	33.5	99.19	0	0.81	17.5
$4f^25d$	e311	3.5	87 400.57 (6)	87 400	0	1.141	$(^1G)^2F$	21.3	99.03	0.01	0.97	12.6
$4f^25d$	e312	3.5	87 539.35 (6)	87 609	−70	0.994	$(^3F)^2G$	38.1	98.96	0.01	1.03	7.60
$4f^25d$	e510	5.5	88 097.78 (10)	88 088	9	1.068	$(^1G)^2H$	39.1	99.19	0.01	0.81	10.5
$4f^25d$	e210	2.5	88 135.24 (10)	88 109	26	1.157	$(^3F)^2D$	37.8	99.15	0	0.84	12.1
$4f^25d$	e411	4.5	88 642.61 (8)	88 687	−45	1.232	$(^3F)^4F$	49.0	98.91	0	1.09	7.37
$4f^25d$	e412	4.5	89 329.54 (8)	89 359	−30	1.035	$(^3F)^2G$	44.5	98.90	0.01	1.09	7.11
$4f^25d$	e107	1.5	90 291.23 (12)	90 255	36	0.869	$(^1G)^2D$	62.5	99.09	0	0.91	10.6
$4f^25d$	e211	2.5	90 339.84 (10)	90 306	33	0.896	$(^1G)^2F$	55.6	99.05	0.02	0.93	7.67
$4f^25d$	e607	6.5	90 380.51 (9)	90 319	61	1.081	$(^1G)^2I$	69.7	99.04	0	0.96	6.48
$4f^25d$	e413	4.5	91 028.86 (9)	91 078	−50	1.015	$(^3F)^2G$	30.6	99.02	0.01	0.97	8.44
$4f^25d$	e511	5.5	91 497.12 (08)	91 520	−24	1.078	$(^3F)^2H$	57.3	98.98	0	1.02	7.89
$4f^25d$	e313	3.5	92 892.71 (10)	92 865	27	1.116	$(^1G)^2F$	33.2	98.98	0.01	1.01	7.26
$4f^25d$	e004	0.5	93 192.73 (21)	93 051	141	1.550	$(^1D)^2S$	55.7	99.19	0	0.81	10.5
$4f^25d$	e108	1.5	93 909.73 (16)	93 839	70	1.305	$(^1D)^2P$	69.8	98.97	0	1.03	10.8
$4f^25d$	e005	0.5	96 293.32 (15)	96 329	−36	1.153	$(^1D)^2P$	58.5	99.08	0	0.91	8.77
$4f^25d$	e212	2.5	96 381.38 (15)	96 392	−10	0.943	$(^1D)^2F$	48.6	98.85	0.01	1.14	13.4
$4f^25d$	e314	3.5	96 560.31 (9)	96 509	51	0.955	$(^1D)^2G$	52.4	98.83	0	1.17	8.50
$4f^25d$	e109	1.5	96 877.38 (12)	96 818	59	0.943	$(^3P)^4F$	28.5	98.90	0	1.10	8.46
$4f^25d$	e110	1.5	97 727.22 (13)	97 696	31	0.725	$(^3P)^4F$	65.8	98.85	0.01	1.14	7.73
$4f^25d$	e414	4.5	98 017.24 (15)	98 011	5	1.148	$(^1D)^2G$	58.2	98.85	0	1.15	8.24
$4f^25d$	e608	6.5	9834.7.09 (9)	98 370	−24	1.009	$(^1I)^2I$	50.7	99.03	0	0.97	6.00
$4f^25d$	e006	0.5	98 541.35 (18)	98 572	−31	1.983	$(^3P)^4P$	64.5	99.08	0	1.13	6.78
$4f^25d$	e512	5.5	98 676.42 (11)	98 614	62	0.945	$(^1I)^2I$	85.2	99.08	0	0.85	7.62
$4f^25d$	e213	2.5	99 033.19 (14)	99 012	21	1.072	$(^3P)^4F$	70.8	99.08	0	1.18	8.66
$4f^25d$	e315	3.5	99 195.97 (10)	99 259	−64	1.137	$(^1D)^2F$	33.1	98.84	0.01	1.16	11.0
$4f^25d$	e214	2.5	99 409.66 (12)	99 435	−25	1.317	$(^3P)^4P$	45.2	98.82	0	1.14	13.4
$4f^25d$	e111	1.5	99 414.87 (10)	99 429	−15	1.210	$(^1D)^2D$	39.9	98.83	0	1.16	7.36
$4f^25d$	e704	7.5	10 0835.39 (11)	100 884	−49	1.049	$(^1I)^2K$	75.1	98.85	0	1.15	5.03
$4f^25d$	e316	3.5	10 0976.62 (11)	100 975	1	1.217	$(^3P)^4F$	52.6	98.79	0.01	1.20	11.3
$4f^25d$	e007	0.5	10 1075.79 (18)	101 004	72	0.827	$(^3P)^4D$	43.5	98.82	0	1.17	8.61
$4f^25d$	e609	6.5	10 1159.67 (13)	101 136	23	1.003	$(^1I)^2K$	46.6	98.99	0	1.01	5.34
$4f^25d$	e215	2.5	10 1586.15 (12)	101 591	−5	1.380	$(^3P)^4P$	41.2	98.77	0	1.23	7.62
$4f^25d$	e112	1.5	10 1900.99 (11)	101 903	−2	1.315	$(^3P)^4D$	57.3	98.75	0	1.25	9.48
$4f^25d$	e415	4.5	10 2038.54 (12)	102 112	−74	1.028	$(^1I)^2H$	64.8	98.78	0.07	1.15	7.62
$4f^25d$	e513	5.5	10 2242.87 (13)	102 305	−62	1.071	$(^1I)^2H$	81.2	98.85	0.05	1.10	7.31

Table 2. (Continued.)

Conf.	Label	J	E_{exp} (unc.)	E_{th}	ΔE	g_L	First LS	comp. %	f^2d %	f^2s %	p^5 f^3d %	τ (ns)
4f^{2}5d	e008	0.5		102 519		0.485	$(^3P)^4D$	47.7	98.85	0	1.15	11.3
4f^{2}5d	e416	4.5	10 2627.40 (10)	102 679	−52	1.178	$(^3P)^4F$	52.1	98.82	0.03	1.14	8.01
4f^{2}5d	e705	7.5	10 2756.25 (11)	102 697	59	0.960	$(^1I)^2L$	84.5	99.04	0	0.96	98.5
4f^{2}5d	e113	1.5	103 403.45 (13)	103 302	101	1.273	$(^3P)^2P$	32.7	98.86	0.01	1.13	51.6
4f^{2}5d	e216	2.5	103 385.28 (14)	103 415	−30	1.336	$(^3P)^4D$	74.2	98.68	0	1.32	44.3
4f^{2}5d	e802	8.5	104 775.22 (22)	104 768	6	1.059	$(^1I)^2L$	98.8	99.06	0	0.94	76.0
4f^{2}5d	e317	3.5	104 888.37 (16)	104 921	−34	1.386	$(^3P)^4D$	82.4	98.67	0	1.33	46.2
4f^{2}5d	e318	3.5	107 900.68 (08)	107 927	−27	1.141	$(^3P)^2F$	76.7	98.65	0.04	1.31	97.2
4f^{2}5d	e217	2.5	108 156.67 (11)	108 107	49	0.877	$(^3P)^2F$	70.8	98.59	0.04	1.37	74.9
4f^{2}5d	e417	4.5	109 414.69 (10)	109 366	48	1.104	$(^1I)^2G$	91.3	98.65	0.05	1.30	78.5
4f^{2}6s	e319	3.5	110 056.47 (5)	110 044	12	0.673	$(^3H)^4H$	96.9	0.01	99.87	0.11	1190
4f^{2}6s	e418	4.5	110 634.11 (4)	110 612	22	0.952	$(^3H)^4H$	58.9	0.10	99.78	0.11	3600
4f^{2}5d	e320	3.5	110 926.84 (11)	110 947	−21	0.890	$(^1I)^2G$	96.1	98.68	0.01	1.31	59.9
4f^{2}5d	e114	1.5	112 658.14 (13)	112 675	−17	0.806	$(^3P)^2D$	86.8	98.70	0.01	1.29	43.5
4f^{2}5d	e218	2.5	113 010.89 (10)	113 026	−15	1.185	$(^3P)^2D$	84.0	98.72	0.01	1.27	59.8
4f^{2}6s	e514	5.5	113 118.93 (4)	113 094	25	1.127	$(^3H)^4H$	84.3	0.02	99.87	0.11	2830
4f^{2}6s	e419	4.5	113 461.85 (4)	113 435	26	0.934	$(^3H)^2H$	59.7	0.07	99.82	0.11	5190
4f^{2}6s	e610	6.5	115 767.20 (5)	115 757	10	1.231	$(^3H)^4H$	99.5	0	99.89	0.11	2100
4f^{2}6s	e115	1.5	115 904.51 (7)	115 904	0	0.409	$(^3F)^4F$	97.3	0.01	99.88	0.11	2490
4f^{2}6s	e219	2.5	116 375.04 (5)	116 370	5	0.988	$(^3F)^4F$	71.0	0.04	99.85	0.11	4230
4f^{2}6s	e515	5.5	116 697.38 (6)	116 684	13	1.097	$(^3H)^2H$	84.0	0.06	99.83	0.11	8920
4f^{2}6s	e321	3.5	117 912.91 (4)	117 928	−16	1.224	$(^3F)^4F$	92.2	0.01	99.88	0.11	4880
4f^{2}6s	e420	4.5	118 448.53 (4)	118 506	−58	1.259	$(^3F)^4F$	67.8	0.01	99.88	0.11	4920
4f^{2}6s	e220	2.5	118 482.80 (5)	118 484	−2	0.906	$(^3F)^2F$	71.7	0.06	99.83	0.11	5490
4f^{2}6s	e322	3.5	119 133.54 (4)	119 178	−45	1.035	$(^3F)^2F$	58.3		99.82	0.11	1360
4f^{2}6s	e421	4.5	122 515.64 (5)	122 521	−6	1.180	$(^1G)^2G$	66.3	0.01	99.89	0.11	2460
4f^{2}6s	e323	3.5	122 854.37 (5)	122 862	−7	1.004	$(^1G)^2G$	55.0	0.03	99.89	0.11	1580
4f^{2}6s	e221	2.5		130 877		1.238	$(^1D)^2D$	86.0	0.01	99.89	0.12	643
4f^{2}6s	e116	1.5		130 953		0.846	$(^1D)^2D$	88.5	0.02	99.89	0.12	590
4f^{2}5d	e117	1.5		132 812		0.800	$(^1S)^2D$	92.9	98.69	0.02	1.29	7.95
4f^{2}5d	e222	2.5		135 004		1.200	$(^1S)^2D$	96.0	98.74	0	1.26	7.81
4f^{2}6s	e009	0.5		135 029		2.538	$(^3P)^4P$	92.6	0	99.89	0.12	812
4f^{2}6s	e118	1.5		135 841		1.702	$(^3P)^4P$	92.3	0	99.89	0.12	780
4f^{2}6s	e611	6.5	136 316.05 (6)	136 305	10	1.078	$(^1I)^2I$	99.5	0	99.89	0.12	689
4f^{2}6s	e516	5.5	136 316.07 (6)	136 308	8	0.924	$(^1I)^2I$	99.5	0	99.89	0.12	677
4f^{2}6s	e010	0.5		136 702		0.798	$(^3P)^2P$	93.2	0.02	99.89	0.12	253
4f^{2}6s	e223	2.5	137 456.40 (11)	137 454	2	1.556	$(^3P)^4P$	88.6	0	99.89	0.12	847
4f^{2}6s	e119	1.5		138 405		1.311	$(^3P)^2P$	86.0	0	99.89	0.12	264
5p^{5}4f^{3}5d		4.5		163 496		0.561	$(^4I)^6K$	70.2	0	0	100	
5p^{5}4f^{3}5d		5.5		165 457		0.847	$(^4I)^6K$	63.4	0	0	100	
4f^{2}6s	e011	0.5		167 690		2.002	$(^1S)^2S$	98.7	0	99.89	0.11	521

In the even parity of Nd IV, the group 5p^{6}4f^2(6d+7s), expected above 190 000 cm^{-1}, perturbs marginally the known levels of 5p^{6}4f^2(5d+6s). In the Tm IV spectrum, recently interpreted for the first time by some of us [19], the addition of 5p^{5}4f^{12}5d to the 5p^{6}4f^{11}(5d+6s) basis set, proved to have a notable quenching effect [20] on the 4f^{12}–4f^{11}5d resonance transitions. The same effect is seen in Nd IV where we added the core-excited unknown

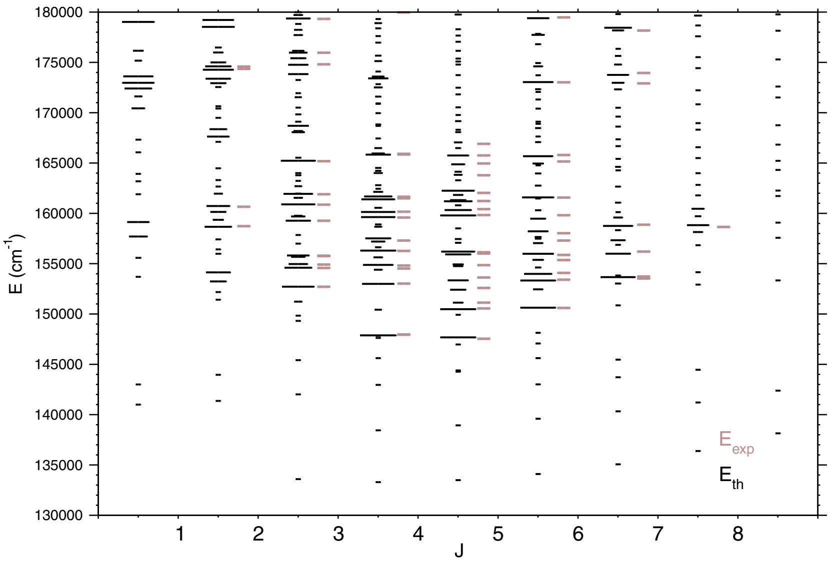

Figure 1. Energy levels of $Nd^{3+}5p^54f^4$ and $5p^64f^26p$. The theoretical levels are represented by bars, the length of which is proportional to the percentage of $5p^64f^26p$. Pure core-excited levels are drawn with the shortest bars. Experimental levels are shown on the right-hand side of the theory.

configuration $5p^54f^35d$ to $5p^64f^2$(5d+6s). Appropriate scaling factors for $5p^54f^35d$ were determined as was done for $5p^54f^4$. In the fitting process, all the CI parameters between $5p^64f^25d$, $5p^64f^26s$ and $5p^54f^35d$ were reduced to a single adjustable one, by means of the ratios of the HFR values. Except for E_{av} and G^3(fs), all the parameters of $4f^26s$ were also constrained by constant ratios to those of $4f^25d$. The root mean square deviation for 119 known levels of $4f^25d$+$4f^26s$ was improved from 68 to 37 cm^{-1} by extending the basis. The full set of parameters is reported in table 4.

It is recalled that the parametrization in the RCG code [4] includes effective parameters for second order of electrostatic interactions which account for double-excitation only, i.e. α, β, γ parameters for $4f^n$ and 'Slater-forbidden' parameters $F^1(4f, 5d)$, $F^3(4f, 5d)$, $G^2(4f, 5d)$, $G^4(4f, 5d)$ for $4f^n5d$. They are not intended to describe at the second order of perturbation the $5p^64f^25d$–$5p^54f^35d$ interaction which corresponds to a single excitation. It is seen in the columns 8–12 of table 2 that the eigenfunctions of the $5p^64f^25d$ levels contain a negligible amount of $5p^64f^26s$ components, whereas $5p^54f^35d$ admixtures are present in all levels.

The predicted $5p^54f^35d$ configuration covers the energy range from 163 000 to 316 000 cm^{-1}, but its strongest transitions to the ground configuration $5p^6(^1S)4f^3$ arise from the decay of its levels based on the core state $5p^55d\,^1P$. The strong lines of the array merge for all the $4f^3$ levels, in a narrow wavelength region 408–418 Å and their theoretical transition probabilities are larger than for the 4f–5d transitions by more than two orders of magnitude. In spite of limited admixtures of $5p^54f^35d$ in the eigenfunctions of $5p^64f^25d$, the overall effect of the $5p^64f^25d$–$5p^54f^35d$ interaction is to reduce the probabilities for the $5p^64f^3$–$5p^64f^25d$ transitions to almost 50% of their values calculated without core excitation [2]. Similar to La IV for $5p^55d$ and $5p^56s$ [13], the $5p^54f^36s$ and $5p^54f^35d$ configurations should overlap in Nd IV. So far, the effect of the $5p^64f^26s$–$5p^54f^36s$ and $5p^54f^36s$–$5p^54f^35d$ interactions on the low even parity levels of Nd IV has not been investigated.

Table 3. Fitted parameters (in cm^{-1}) for odd parity configurations $4f^3$, $4f^26p$ and $5p^54f^4$ of Nd^{3+} compared with HFR radial integrals. The scaling factors are $SF(P) = P_{fit}/P_{HFR}$. Constraints on some parameters (denoted 'r' in the 'Unc' columns of standars errors) are detailed in the text.

	$4f^3$				$4f^26p$				$5p^54f^4$			
Param. P	P_{fit}	Unc.	P_{HFR}	SF	P_{fit}	Unc.	P_{HFR}	SF	P_{fit}	Unc.	P_{HFR}	SF
E_{av}	25 982	105			164 326	62	131 321		183 474	157	168 502	
$F^2(4f, 4f)$	78 824	317	102 658	0.768	82 532	362	110 783	0.754	73 544	707	96 504	0.762
$F^4(4f, 4f)$	54 044	416	64 418	0.839	61 809	871	69 929	0.884	52 942	800	60 281	0.878
$F^6(4f, 4f)$	36 925	260	46 345	0.797	40 398	1304	50 430	0.801	34 553	r	43 289	0.798
α	6.6	2			19.5	2			19.5	r		
β	−268	66			−495	r			−495	r		
γ	1 256	82			1 614	r			1 614	r		
ζ_f	892	9	957	0.932	984	11	1 059	0.929	789	30	880	0.897
ζ_p					3 576	34	2 962	1.207	16 574	412	16 204	1.023
$F^2(4f, np)$					7 933	270	9 951	0.797	36 213	752	51 106	0.709
$G^2(4f, np)$					2 385	173	2 518	0.947	24 663	824	29 048	0.849
$G^4(4f, np)$					1 925	339	2 313	0.832	16 210	978	22 017	0.736
Configuration Interaction involving $4f^3$												
$4f^3 - 4f^26p$												
$R^2(4f4f, 4f6p)$	−4 755	230	−4 973	0.956								
$R^2(4f4f, 4f6p)$	−3 053	r	−3 193	r								
$5p^64f^3 - 5p^54f^4$												
$R^2(4f5p, 4f4f)$	−20 835	r	−21 791	r								
$R^4(4f5p, 4f4f)$	−11 562	r	−12 092	r								
$R^2(5p5p, 4f5p)$	−37 332	r	−39 045	r								
$4f^3 - 4f5d^2$												
$R^1(4f4f, 5d5d)$	16 928	r	17 705	r								
$R^3(4f4f, 5d5d)$	13 809	r	14 443	r								
$R^5(4f4f, 5d5d)$	10 584	r	11 070	r								

5. Classified lines

In the preparation of the final list of classified lines, the theoretical transition probabilities and observed line intensities were compared systematically. The present intensities are visual estimates of plate blackening over a scale 1–1000 without correction for plate sensitivity. They result from many plates with limited wavelength overlaps and their consistency throughout the 1163–2798 Å range needs improvements. In spite of their large uncertainties (about 30%), these intensity estimates were very useful when searching for new levels.

A straight application of the Ritz combination principle leads to many doubly, and seven triply, classified lines. In several cases, the gA value for one of the multiple classifications is much smaller than the others and we have rejected the less probable classifications. The two levels $J = 11/2, 13/2$ of the $4f^26s^2I$ term are too close to be separated and all their classified lines with odd levels of the same J-values give some of the 90 double classifications in the list of 1426 wavelengths. Examples of classified lines are given in table 5 for the four highest levels of $4f^3$ in the odd parity, and in table 6 for the levels at 75 666 cm^{-1} and 76 411 cm^{-1} in the even parity. A complete version of table 5 (ordered by increasing energies of the odd parity levels) is provided as a supplementary file which is available online (see stacks.iop.org/JPhysB/40/3957). The 1426 classified lines (1531 transitions) ordered by

Table 4. Fitted parameters (in cm^{-1}) for even parity configurations of Nd^{3+} compared with HFR radial integrals. The scaling factors are $SF(P) = P_{fit}/P_{HFR}$. Constraints on some parameters (denoted 'r' in the 'Unc' columns of standars errors) are detailed in the text.

	$4f^2 5d$				$4f^2 6s$				$5p^5 4f^3 5d$	
Param. P	P_{fit}	Unc.	P_{HFR}	SF	P_{fit}	Unc.	P_{HFR}	SF	Adopted	P_{HFR}
E_{av}	89 746	96	55 887		122 722	17	90 977	221 000		196 431
F^2(ff)	83 559	420	109 950	0.760	82 883	r	110 707	0.750	79 884	104 124
F^4(ff)	60 656	1 123	69 359	0.874	61 110	r	69 878	0.874	54 852	65 417
F^6(ff)	40 565	1 285	50 007	0.811	40 866	r	50 392	0.811	37 518	47 086
α	20	1			20	r			22	
β	−561	30			−561	r			−557	
γ	1 243	394			1 243	r			1 817	
ζ_f	988	3	1 052	0.939	994	r	1 059	0.939	901	972
ζ_d	1 124	6	1 146	0.981					1 024	1 047
ζ_p									17 350	17 350
F^1(fd)	758	57								
F^2(fd)	23 356	84	30 830	0.758					22 029	30 248
F^3(fd)	149	122								
F^4(fd)	16 538	133	15 288	1.082					17 034	15 162
F^2(pf)									36 034	51 787
F^2(pd)									40 350	49 631
G^1(fd)	11 294	85	13 343	0.846					10 834	14 201
G^2(fd)	2 012	111								
G^3(fd)	10 836	100	11 355	0.954					11 715	11 677
G^4(fd)	1 757	144								
G^5(fd)	7 374	100	8 788	0.839					7 874	8 956
G^3(fs)					2 732	80	3 365	0.812		
G^2(pf)									22 819	27 437
G^4(pf)									15 873	21 226
G^1(pd)									38 886	58 082
G^3(pd)									28 525	36 258
Configuration Interaction										
$4f^2 5d - 4f^2 6s$										
R^2(fd,fs)	618	22	974	0.634						
R^3(fd,sf)	1 880	r	2 962	r						
$5p^6 4f^2 5d - 5p^5 4f^3 5d$										
R^2(fp,ff)	−12 017	r	−18 933	r						
R^4(fp,ff)	−6 410	r	−10 099	r						
R^2(pp,fp)	−23 878	r	−37 622	r						
R^2(pd,fd)	−16 981	r	−26 754	r						
R^4(pd,fd)	−10 749	r	−16 936	r						
R^1(pd,df)	−15 785	r	−24 870	r						
R^3(pd,df)	−10 999	r	−17 330	r						
$5p^6 4f^2 6s - 5p^5 4f^3 5d$										
R^2(ps,fd)	4 111	r	6 746	r						
R^3(ps,df)	−880	r	−1 386	r						

increasing wavelength are also available on the website of the MOLAT database [21] of the Meudon Observatory.

Some comparisons of intensities versus gA happen to be unsatisfactory and the odd parity levels with $J = 7/2$ at 147 943.06 and 147 964.36 cm^{-1} represent an extreme case

Table 5. Classified lines of Nd IV for the four upper levels of $4f^3$. All experimental energies and wavenumbers σ_{exp} are in cm^{-1}. $\Delta\lambda$ is the difference between experimental λ_{exp} and Ritz calculated wavelengths in Å . The intensities (visual estimates of plate blackening) are followed by D for doubly classified lines. The calculated weighted transition probabilities gA in emission (in 10^6 s^{-1}) are omitted if gA is less than $5(10^5)$.

λ_{exp}	Int	gA	σ_{exp}	$\Delta\sigma$	$\Delta\lambda$	Classif.		E^o	J_o	E^e	J_e
o407	E_{th} = 49 345 cm^{-1}										
1659.966	80	223	60 242.21	−0.03	0.001	o407	e417	49 172.45	4.5	109 414.69	4.5
1702.756	250	791	58 728.32	0.09	−0.003	o407	e318	49 172.45	4.5	107 900.68	3.5
1884.292	80	171	53 070.33	−0.09	0.003	o407	e513	49 172.45	4.5	102 242.87	5.5
1930.345	3	13	51 804.20	0.03	−0.001	o407	e316	49 172.45	4.5	100 976.62	3.5
1999.062	1	14	50 023.46	−0.06	0.002	o407	e315	49 172.45	4.5	99 195.97	3.5
2019.381	2	13	49 504.14	0.17	−0.007	o407	e512	49 172.45	4.5	98 676.42	5.5
2046.632	20	54	48 845.11	0.31	−0.013	o407	e414	49 172.45	4.5	98 017.24	4.5
2109.581	1	2	47 387.74	−0.08	0.005	o407	e314	49 172.45	4.5	96 560.31	3.5
2489.480	40	13	40 156.90	−0.19	0.011	o407	e412	49 172.45	4.5	89 329.54	4.5
2735.657	80	5	36 543.48	−0.18	0.014	o407	e410	49 172.45	4.5	85 716.11	4.5
o306	E_{th} = 50 227 cm^{-1}										
1645.660	80	186	60 765.90	0.01	0.000	o306	e320	50 160.95	3.5	110 926.84	3.5
1724.261	200	633	57 995.85	0.13	−0.004	o306	e217	50 160.95	3.5	108 156.67	2.5
1731.917	5	19	57 739.49	−0.24	0.007	o306	e318	50 160.95	3.5	107 900.68	3.5
1905.978	35	5	52 466.50	0.05	−0.002	o306	e416	50 160.95	3.5	102 627.40	4.5
1927.616	40	109	51 877.56	−0.03	0.001	o306	e415	50 160.95	3.5	102 038.54	4.5
2088.917	10	–	47 856.48	0.19	−0.008	o306	e414	50 160.95	3.5	98 017.24	4.5
2154.524	80	37	46 399.38	0.02	−0.001	o306	e314	50 160.95	3.5	96 560.31	3.5
2674.554	80	4	37 378.31	−0.09	0.006	o306	e312	50 160.95	3.5	87 539.35	3.5
2684.516	40	3	37 239.61	−0.01	0.001	o306	e311	50 160.95	3.5	87 400.57	3.5
2705.321	30	1	36 953.23	0.02	−0.002	o306	e209	50 160.95	3.5	87 114.16	2.5
o307	E_{th} = 68 776 cm^{-1}										
2261.341	150	153	44 207.86	0.13	−0.007	o307	e218	68 803.16	3.5	113 010.89	2.5
2461.611	150	108	40 611.51	−0.02	0.001	o307	e417	68 803.16	3.5	109 414.69	4.5
2540.306	10	7	39 353.68	−0.17	0.012	o307	e217	68 803.16	3.5	108 156.67	2.5
2556.945	100	27	39 097.44	−0.08	0.005	o307	e318	68 803.16	3.5	107 900.68	3.5
o207	E_{th} = 70 093 cm^{-1}										
2320.648	3	15	43 078.18	−0.12	0.006	o207	e218	69 932.59	2.5	113 010.89	2.5
2339.805	80	89	42 725.51	−0.04	0.002	o207	e114	69 932.59	2.5	112 658.14	1.5
2438.630	100	88	40 994.19	−0.06	0.003	o207	e320	69 932.59	2.5	110 926.84	3.5
2615.369	120D	12	38 224.12	0.04	−0.003	o207	e217	69 932.59	2.5	108 156.67	2.5
2632.997	200	2	37 968.21	0.12	−0.008	o207	e318	69 932.59	2.5	107 900.68	3.5

of disagreement. These two levels have a theoretical separation three times larger than the experimental one and are almost pure $4f^26p$ and $5p^54f^4$, respectively (see table 1). However, their classified lines have comparable intensities and a larger mixing might be expected. The level with $J = 13/2$ at 153 530.33 cm^{-1}, and the adjacent $4f^26p$ level at 153 724.25 cm^{-1} (see table 1), present the same underestimated mixing. Thus, the wavefunctions of high odd parity levels indicate that, for eventual plasma diagnostics, the $4f^3$–$4f^25d$ transitions rather than the $4f^26s$–$4f^26p$ transitions should be used. In spite of a few exceptions, the classified lines grouped by levels show a qualitative agreement of intensities with theoretical transition probabilities in tables 5 and 6. The lifetimes calculated from theoretical gA values are reported for all $4f^25d$ and $4f^26s$ levels in the last column of table 2.

Table 6. Classified lines of Nd IV for two selected levels of $4f^25d$. All experimental energies and wavenumbers σ_{exp} are in cm^{-1}. $\Delta\lambda$ is the difference between experimental λ_{exp} and Ritz calculated wavelengths in Å . The intensities (visual estimates of plate blackening) are followed by D for doubly classified lines. The calculated weighted transition probabilities gA in emission (in 10^6 s^{-1}) are omitted if gA is less than $5(10^5)$.

λ_{exp}	Int	gA	σ_{exp}	$\Delta\sigma$	$\Delta\lambda$	Classif.		E^o	J_o	E^e	J_e
e302	E_{th}= 75 705 cm^{-1}										
1196.176	15	430	83 599.76	0.13	−0.002	o221	e302	159 266.54	2.5	75 666.91	3.5
1240.608	10	–	80 605.65	−0.13	0.002	o320	e302	156 272.69	3.5	75 666.91	3.5
1244.681	3	–	80 341.90	0.32	−0.005	o421	e302	156 008.49	4.5	75 666.91	3.5
1248.020	20	–	80 126.90	−0.25	0.004	o218	e302	155 794.06	2.5	75 666.91	3.5
1261.867	5	–	79 247.63	−0.27	0.004	o216	e302	154 914.81	2.5	75 666.91	3.5
1263.498	150	954	79 145.34	0.00	0.000	o318	e302	154 812.25	3.5	75 666.91	3.5
1267.199	40	284	78 914.18	0.09	−0.001	o215	e302	154 581.00	2.5	75 666.91	3.5
1268.201	2	–	78 851.84	0.38	−0.006	o317	e302	154 518.37	3.5	75 666.91	3.5
1282.682	20	115	77 961.62	0.24	−0.004	o418	e302	153 628.29	4.5	75 666.91	3.5
1292.804	150	2 049	77 351.27	−0.04	0.001	o316	e302	153 018.22	3.5	75 666.91	3.5
1297.965	20	279	77 043.67	0.28	−0.005	o214	e302	152 710.30	2.5	75 666.91	3.5
1321.582	100	92	75 666.87	−0.04	0.001	o401	e302	0.00	4.5	75 666.91	3.5
1335.225	80	1 562	74 893.76	0.12	−0.002	o415	e302	150 560.55	4.5	75 666.91	3.5
1391.248	1	–	71 877.92	−0.06	0.001	o413	e302	147 544.89	4.5	75 666.91	3.5
1589.340	250	160	62 919.17	0.20	−0.006	o201	e302	12 747.94	2.5	75 666.91	3.5
1614.278	60	21	61 947.18	0.09	−0.002	o301	e302	13 719.82	3.5	75 666.91	3.5
1723.782	100	49	58 011.96	0.16	−0.005	o302	e302	17 655.11	3.5	75 666.91	3.5
1781.703	120	42	56 126.07	−0.04	0.001	o303	e302	19 540.80	3.5	75 666.91	3.5
1795.424	5	4	55 697.14	0.02	−0.001	o404	e302	19 969.79	4.5	75 666.91	3.5
1845.919	2	5	54 173.56	0.04	−0.001	o405	e302	21 493.39	4.5	75 666.91	3.5
1948.037	3	3	51 333.72	−0.09	0.003	o203	e302	24 333.10	2.5	75 666.91	3.5
2769.387	5	0	36 098.41	−0.08	0.006	o206	e302	39 568.42	2.5	75 666.91	3.5
e403	E_{th} = 76 406 cm^{-1}										
1266.607	5	–	78 951.12	−0.23	0.004	o517	e403	155 363.07	5.5	76 411.72	4.5
1275.499	20	130	78 400.72	0.19	−0.003	o318	e403	154 812.25	3.5	76 411.72	4.5
1295.052	5	125	77 216.99	0.42	−0.007	o418	e403	153 628.29	4.5	76 411.72	4.5
1298.797	8	261	76 994.31	−0.22	0.004	o514	e403	153 406.25	5.5	76 411.72	4.5
1305.372	40	469	76 606.51	0.01	0.000	o316	e403	153 018.22	3.5	76 411.72	4.5
1308.698	100	63	76 411.85	0.13	−0.002	o401	e403	0.00	4.5	76 411.72	4.5
1312.656	8	159	76 181.41	0.21	−0.004	o417	e403	152 592.92	4.5	76 411.72	4.5
1342.014	300	1 243	74 514.90	0.29	−0.005	o501	e403	1 897.11	5.5	76 411.72	4.5
1347.792	150	1 419	74 195.42	−0.18	0.003	o512	e403	150 607.32	5.5	76 411.72	4.5
1348.637	120	4 007	74 148.95	0.12	−0.002	o415	e403	150 560.55	4.5	76 411.72	4.5
1572.043	2	10	63 611.51	0.08	−0.002	o402	e403	12 800.29	4.5	76 411.72	4.5
1595.099	30	16	62 692.05	0.15	−0.004	o301	e403	13 719.82	3.5	76 411.72	4.5
1659.745	1D	3	60 250.21	0.02	−0.001	o502	e403	16 161.53	5.5	76 411.72	4.5
1701.928	120	61	58 756.88	0.27	−0.008	o302	e403	17 655.11	3.5	76 411.72	4.5
1758.365	120	88	56 871.00	0.08	−0.002	o303	e403	19 540.80	3.5	76 411.72	4.5

6. Comparison with earlier work by Irwin

At the end of the present work, we re-examined Irwin's Nd IV analysis [10] which we had initially rejected [2] on the basis of an erroneous ground term $4f^3$ ^4I derived from 12 4f–5d transitions. As a matter of fact, Irwin's classified lines connecting the ^3H_J core levels of $4f^26s$ with those of $4f^26p$ were partly correct, at least for the splittings of the $4f^2(^3H_J)6s$

doublets with $J = 5, 6$. The different transition arrays were not connected and were reported separately with the lowest $4f^2 6s$ level within each array arbitrarily set at 100 000 cm^{-1}. In the array built on $4f^2(^3H_5)$, Irwin gave two tentative levels of $4f^2(^3H_5)5d$ at 64 793.18 and 68 036 cm^{-1}, which we confirmed. Their energies relative to the ground level are, respectively, 77 912.20 and 81 155.16 cm^{-1}. About 87% of the selected strong lines below 2000 Å published in [10] are now classified. Our present tables 5 and 6 give 67 classified lines, from which 40 were in the wavelength list of [10], with a mere three lines classified as transitions from $4f^2 6p$ to $4f^2 5d$. The peak currents (200 and 400 A) used in [10] obviously favoured $4f^3$–$4f^2 5d$ transitions below 2000 Å. A number of unclassified lines in Irwin's selection above 2000 Å might belong to Nd III.

7. Conclusion

The first analysis of the Nd IV emission spectrum, observed at the NIST and at the Observatoire de Paris-Meudon, led to the determination of the entire ground configuration $4f^3$ and to a large part of the excited configurations $4f^2 5d$, $4f^2 6s$ and $4f^2 6p$ with the support of predictions using the Cowan codes [4]. A number of odd levels of $4f^2 6p$ have a large percentage of components of $5p^5 4f^4$. For 23 of the upper odd parity levels, this core-excited configuration is dominant. In the even parity, the lowest core-excited configuration $5p^5 4f^3 5d$ is still unknown, but its addition to $5p^6 4f^2(5d + 6s)$ in a three-configurations basis improves significantly the calculated energies and reduces the transition probabilities for $5p^6 4f^3$–$5p^6 4f^2 5d$ by a factor of about two. It is hoped that the present theoretical predictions of lifetimes will stimulate new experiments. Also, absorption spectra using the same technique as for Ba^{2+} [22] or La^{3+} [23] might help to locate the $5p^6 4f^3$–$5p^5 4f^3 5d$ very strong transitions around 410 Å. This is an important issue in the study of radiative properties for Nd^{3+}.

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Appendix

The classified lines of Nd IV are ordered by increasing energies of the odd parity levels, then by increasing wavelength for each level in the supplementary file, accessible online at stacks.iop.org/JPhysB/40/3957.

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