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Theoretical Investigation of the Odd Configurations of Ni II.*

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Two groups of odd levels in Ni II were investigated: those belonging to the complex $3d^84p+3d^74s4p+3d^85p$ and those belonging to the configuration $3d^84f$. In the first group the calculated positions of the levels were fit to the positions of the 174 observed levels with an rms error of 133 cm^{-1}. The fit for the second group was based on 60 observed levels and had an rms error of 25 cm^{-1}. The predictions of this investigation helped in the discovery of many of the observed levels.

Key words: Energy levels; *g*-factors; nickel; parameters, theory.

1. Introduction

The configuration $3d^84p$ has been well known, and many of its observed levels have been reported in AEL [1].[1] Theoretical interpretations of the $3d^84p$ level structure were performed by various investigators [2–4].

About four years ago Professor A. G. Shenstone informed us of some newly discovered odd levels, presumably belonging to the configurations $3d^74s4p$, $3d^85p$, and $3d^8nf$ ($n=4$, 5, 6, 7). This paper is the result of his suggestion that a theoretical investigation of these configurations be made to help him with his experimental investigation. The companion paper containing Shenstone's experimental results has already been published [5].

Our calculations involved the diagonalization of the energy matrices of the $3d^84p$, $3d^74s4p$, and $3d^85p$ configurations calculated as one complex, and the energy tions calculated as one complex, and the energy matrices associated with the $3d^84f$ configuration. In the case of the $3d^84p+3d^74s4p+3d^85p$ complex, we were able to fit the 174 observed levels to the calculated ones with an rms error of 133 cm^{-1}. For the $3d^84f$ configuration, the 60 observed levels could be fitted to the calculated ones with an rms error of 25 cm^{-1}. All the levels were designated in a well defined coupling scheme.

2. Notations and Definitions

In the text and tables Slater parameters and spin-orbit parameters are designated in the usual way. Other symbols and abbreviations used in the text have the following meanings:

B, C = linear combinations of Slater parameters $F_2(dd)$ and $F_4(dd)$; (see, for example, ref. [7]).

α, β, T = effective interactions among d electrons; [9].

H, J, K = parameters of configuration interaction which are appropriate linear combinations of Slater integrals; (see, for example, refs. [4] and [8]).

Δ = root mean square error ("rms error").

"Diag.", "L.S." = abbreviations for "Diagonalization" and "Least-squares calculation," respectively.

In cases where several configurations have analogous parameters, the configuration is also explicitly specified.

3. The Theoretical Interpretation of the Configurations $3d^84p+3d^74s4p+3d^85p$

We shall use the following abbreviations:

$$d^8p=3d^84p,$$

$$d^7sp=3d^74s4p,$$

$$d^8p'=3d^85p.$$

In his first letter, Professor Shenstone supplied us with 17 levels belonging to the d^7sp configuration; 9 of them were low and were assumed to be based on $d^7s(^5F)$; 8 of them were high and it was supposed that they were based on d^7s (^3P).

In the first stage of our calculations only the two configurations d^8p+d^7sp were included. The interaction parameters of d^8p are well known [2–4]. For an estimate of initial parameters for d^7sp, we were able to use analogous calculations performed by C. Roth [4] on the Cu II and Zn II spectra and by A. Schwimmer [6] on Sc II, Ti II and V II. It is well known

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[1] Figures in brackets indicate the literature references at the end of this paper.

from works on the even configurations in the iron group [7, 8] and from reference (4) that the electrostatic interaction parameters change linearly along sequences of spectra with constant ionization. The behavior of D', defined as the separation between the centers of the configurations $d^{n-1}sp$ and $d^{n}p$, and the behavior of the spin-orbit interaction parameters are also approximately linear.

Hence we could interpolate the values of D' and the d-p interaction parameters from the spectra of Sc II, Ti II, V II, Cu II, and Zn II mentioned above. For the G_1 (sp) parameter we could rely upon the spectra of the right hand side of the period. Values for the parameters B, C, G_2 (ds) and H were simply taken from the even configurations of Ni II [10]. J and K were also extrapolated from the right hand side of the period.

The first diagonalization was performed using the described above parameters. The nine low observed levels of Shenstone's first list were quartets. It also became evident that the correct coupling for the d^7sp configuration is the following: first the s and p electrons are coupled and then the resulting term is coupled with a term of d^7. Such a coupling was already used by C. Roth [4]. Using this scheme we found that all the nine low-lying levels reported by Shenstone are based on the combination $d^7(^4F)sp(^3P)$.

After our initial diagonalization, additional observed levels were provided by Professor Shenstone to bring the total number of observed levels which were fitted to calculated levels of d^8p+d^7sp up to 78. In the final least-squares calculation based on the previously described interaction parameters, 43 levels were found to belong to the d^8p configuration and 35 to the new configuration d^7sp. The rms error was 100 cm^{-1} for the calculated levels.

The observed levels in the range 110,000–120,000 cm^{-1} could not be satisfactorily fitted in the previous diagonalization. The reason for this was rather clear: in the same energy range some levels belonging to the d^8p' configuration were also observed. This means that in order to obtain good results, one has to include the interaction between the configurations d^7sp and d^8p' as well. Because such an extended calculation requires quite a number of additional new parameters, we first performed a separate calculation on the d^8p' configuration in which we included only the levels which we believed not to be strongly perturbed by d^7sp. This auxiliary calculation provided initial values for the $3d-5p$ interaction parameters and for ζ_{5p}; for B and C we used the same values as for the d^8p configuration.

The extended energy matrix of the three configurations was diagonalized using the approximated values for the parameters found in the previous calculations and estimates for the initial values for J' and K'. In the subsequent least-squares calculations we gradually fitted more and more observed levels to the calculated ones and reached a stage at which 109 observed levels were fitted unequivocally to the calculated ones with an rms error of 70 cm^{-1}. A considerable improvement of the fit between the observed and calculated levels was achieved in the previously problematic range 110,000–120,000 cm^{-1}.

These results enabled Professor Shenstone to supply us with an improved and extended list of observed levels. This new list of levels was used in a new series of iterated diagonalizations. In the final least-squares calculation of this stage, which included the effective-interaction parameters β and T, 132 levels were fit with an rms error of 112 cm^{-1}.

We were not able to include in the fit ten levels of the experimental list. Of these levels, seven were considered by Professor Shenstone to be of doubtful identification. The inclusion of any of the remaining three in the least-squares calculation increases the rms error considerably and forces some of the parameters to assume unreasonable values.

In subsequent correspondence with Professor Shenstone a final level list was constructed. The ten problematical levels were reassigned—some to other configurations and others to different J values. Also, the list was amended by addition of 40 new levels to bring the total up to 174. A new iteration was performed, and the observed levels were fitted to the calculated values with an rms error of 133 cm^{-1}. The parameters of this final calculation are given in table 1, Column L.S. 1a.

The parameters β and T could not both be derived directly from the least squares calculation. Instead, the value of T was fixed at a value obtained from our calculations on the even third spectra of the iron group [8]. When T and β were not included in the calculation, the rms error increased to 145 cm^{-1} as indicated in table 1, column L.S. 2.

Table 2 contains the list of observed and calculated levels of the configurations $d^8p+d^7sp+d^8p'$. The spectral purities of the reported assignments are given only when at least one level of the term has a purity of less than 60 percent. In a few cases the parent term was strongly mixed and was not included in the designation. Four observed levels which were assigned to these configurations by Professor Shenstone could not be fit into the scheme on calculated levels. They are:

1) The level $d^7sp\,^2D_{5/2}$ observed at 135258.88 cm^{-1} with a deviation of about 600 cm^{-1} from the calculated value;
2) the levels $d^7sp\,^4P_{5/2}$ 131834.94 cm^{-1}
   $^4P_{3/2}$ 132225.15 cm^{-1}
   $^4P_{1/2}$ 132120.70 cm^{-1}

which differ from the calculated values by about 1,200 cm^{-1}. When these levels are included in the iterative fitting procedure, the ^4P levels disagree by about 700 cm^{-1} and the mean error increases to 188 cm^{-1}. (See table 1, column L.S. 1b; these levels are those in table 2 which are enclosed by parentheses.)

4. The Theoretical Interpretation of the Configuration $3d^84f$

The abbreviation d^8f will be used for the configuration $3d^84f$. The treatment of this configuration was relatively simple. Initial values for the parameters B, C, and ζ_d were taken from the configuration d^8 of Ni III. [8] A rough first estimate for the parameters

TABLE 1. *Parameters of the configurations* $d^8p+d^7sp+d^8p$.

All values are in units of cm^{-1}

P	Diag. 1	L.S. 1a	L.S. 1b	Diag. 2	L.S. 2
$A(3d^74s4p)$	120990	120980 ± 80	120775 ± 110	120830	120815 ± 85
$A(d^7sp)-A(3d^84p)$	58350	58335 ± 105	58170 ± 145	58540	58500 ± 120
$A(d^7sp)-A(3d^85p)$	7785	7755 ± 95	7550 ± 130	7950	7940 ± 100
$B-d^7sp$	1113	1112 ± 3	1108 ± 4	1130	1131 ± 3
$B-d^8p$	1046	} 1047 ± 4	} 1046 ± 5	1073	} 1075 ± 4
$B-d^8p'$	1046			1073	
$C-d^7sp$	4875	4888 ± 23	4928 ± 31	4550	4550 ± 14
$C-d^8p$	4535	} 4547 ± 27	} 4549 ± 37	4170	} 4172 ± 28
$C-d^8p'$	4535			4170	
$G_2(ds)-d^7sp$	1755	1756 ± 30	1752 ± 42	1770	1751 ± 32
$F_2(dp)-d^7sp$	478	477 ± 6	455 ± 8	478	481 ± 6
$F_2(dp)-d^8p$	352	353 ± 5	353 ± 8	352	351 ± 7
$F_2(dp)-d^8p'$	87	85 ± 7	87 ± 10	87	87 ± 8
$G_1(sp)-d^7sp$	10220	10192 ± 31	10076 ± 42	10290	10306 ± 34
$G_1(dp)-d^7sp$	359	362 ± 9	353 ± 13	346	352 ± 12
$G_1(dp)-d^8p$	295	293 ± 6	296 ± 8	300	299 ± 7
$G_1(dp)-d^8p'$	88	88 ± 7	90 ± 10	97	98 ± 9
$G_3(dp)-d^7sp$	42	} 42 ± 3	} 43 ± 3	40	} 41 ± 3
$G_3(dp)-d^8p$	42			40	
$G_3(dp)-d^8p'$	7	8 ± 4	8 ± 5	8	9 ± 4
α	29	27 ± 3	28 ± 4	78	76 ± 2
β	−900	−1230 ± 160	−1370 ± 230	....	....
T	−5.7	Fixed	Fixed	....	....
H d^7sp-d^8p	185	220 ± 40	175 ± 55	120	135 ± 55
J d^7sp-d^8p	1650	1830 ± 330	1755 ± 465	1300	1290 ± 370
J d^7sp-d^8p'	400	410 ± 80	475 ± 110	485	465 ± 85
K d^7sp-d^8p	2850	2620 ± 370	2730 ± 525	2965	2875 ± 425
K d^7sp-d^8p'	1035	1005 ± 75	1015 ± 110	1070	1050 ± 85
ζ_d-d^7sp	749	744 ± 21	748 ± 29	749	748 ± 23
ζ_d-d^8p	663	} 662 ± 18	} 664 ± 25	663	} 657 ± 20
ζ_d-d^8p'	663			663	
ζ_p-d^7sp	630	640 ± 70	720 ± 100	595	605 ± 75
ζ_p-d^8p	455	450 ± 50	450 ± 75	455	450 ± 55
ζ_p-d^8p'	140	130 ± 55	130 ± 75	155	135 ± 60
Δ		133 cm^{-1}	188 cm^{-1}		145 cm^{-1}
Number of levels		174	178		174

TABLE 2. Ni II—*Observed and calculated energy levels* $3d^84p+3d^85p+3d^74s4p$ *in units of* cm^{-1}

THEORETICAL ASSIGNMENT		J	OBS.	CALC.	O−C	CALC. g
MAIN COMPONENT	ADDITIONAL					
$3d^8(^3F)4p\,^4D$		7/2	51557.85	51701	−143	1.423
		5/2	52738.45	52846	−108	1.359
		3/2	53634.62	53721	−86	1.187
		1/2	54176.26	54252	−76	.003
$3d^8(^3F)4p\,^4G$		11/2	53496.49	53364	132	1.273
		9/2	53365.17	53367	−2	1.180
		7/2	54262.63	54205	58	1.021
		5/2	55018.71	54931	88	.620
$3d^8(^3F)4p\,^4F$		9/2	54557.05	54523	34	1.288
		7/2	55417.83	55342	76	1.185
		5/2	56075.26	55990	85	.987
		3/2	56424.49	56352	72	.423
$3d^8(^3F)4p\,^2G$		9/2	55299.65	55315	−15	1.148
		7/2	56371.44	56478	−107	.936
$3d^8(^3F)4p\,^2F$		7/2	57080.55	57103	−22	1.119
		5/2	58493.21	58471	22	.934
$3d^8(^3F)4p\,^2D$		5/2	57420.16	57376	44	1.132
		3/2	58705.95	58647	59	.797

TABLE 2. Ni II—*Observed and calculated energy levels* 3d⁸4p + 3d⁸5p + 3d⁷4s4p *in units of* cm^{-1}—Continued

THEORETICAL ASSIGNMENT		J	OBS.	CALC.	O–C	CALC. g
MAIN COMPONENT	ADDITIONAL					
$3d^8(^3P)4p\,^4P$		5/2	66571.35	66599	−28	1.487
		3/2	66579.71	66584	−4	1.564
		1/2	67031.02	66998	33	2.267
$3d^8(^1D)4p\,^2F$		5/2	67694.64	67666	29	.938
		7/2	68131.21	68053	78	1.179
$3d^8(^1D)4p\,^2D$		3/2	68154.31	68235	−81	1.050
		5/2	68735.98	68796	−60	1.258
$3d^8(^1D)4p\,^2P$		1/2	68281.62	68118	164	1.070
		3/2	68965.65	68831	135	1.264
$3d^8(^3P)4p\,^4D$		7/2	70778.11	70759	19	1.390
		5/2	70635.55	70626	10	1.334
		3/2	70706.74	70672	35	1.189
		1/2	70748.66	70718	31	.012
$3d^8(^3P)4p\,^2D$		5/2	71770.83	71909	−138	1.206
		3/2	72375.42	72449	−74	.850
$3d^8(^3P)4p\,^2P$		3/2	72985.65	72963	23	1.309
		1/2	73903.25	73886	17	.926
$3d^8(^3P)4p\,^2S$		1/2	74283.33	74399	−116	1.721
$3d^8(^3P)4p\,^4S$		3/2	74300.93	74304	−3	1.968
$3d^8(^1G)4p\,^2H$		9/2	75149.55	75190	−40	.910
		11/2	75721.71	75705	17	1.091
$3d^8(^1G)4p\,^2F$		7/2	75917.61	75977	−59	1.143
		5/2	76402.04	76395	7	.858
$3d^8(^1G)4p\,^2G$		7/2	79823.03	79874	−51	.890
		9/2	79923.88	79977	−53	1.110
$3d^7(^4F)\,^4sp(^3P)\,^6F$		11/2	86343.21	86645	−302	1.450
		9/2	86870.03	86956	−86	1.458
		7/2	87538.09	87599	−61	1.417
		5/2	88128.56	88170	−41	1.332
		3/2	88582.01	88608	−26	1.084
		1/2	88881.59	88884	−2	−.619
$3d^7(^4F)sp(^3P)\,^6D$		9/2	88171.88	88272	−100	1.519
		7/2	89100.47	89213	−113	1.541
		5/2		89900		1.590
		3/2		90374		1.742
		1/2		90654		3.285
$3d^7(^4F)sp(^3P)\,^6G$		13/2		88787		1.384
		11/2	89460.35	89327	133	1.345
		9/2	89918.47	89795	123	1.281
		7/2	90275.30	90164	111	1.164
		5/2	90526.18	90428	98	.903
		3/2		90595		.106
$3d^7(^4F)sp(^3P)\,^4F$		9/2	94283.94	94262	22	1.295
		7/2	94705.93	94701	5	1.214
		5/2	95332.53	95324	9	1.001
		3/2	95893.76	95878	16	.423
$3d^7(^4F)sp(^3P)\,^4G$		11/2	94396.74	94363	34	1.274
		9/2	95017.71	94989	29	1.208
		7/2	95573.39	95572	1	1.027
		5/2	96052.48	96056	−4	.625
$3d^7(^4F)sp(^3P)\,^4D$		7/2	96535.87	96629	−93	1.407
		5/2	97273.83	97376	−102	1.346
		3/2	97799.66	97917	−117	1.178
		1/2	98122.63	98250	−127	.003

TABLE 2. Ni II—*Observed and calculated energy levels* 3d⁸4p + 3d⁸5p + 3d⁷4s4p *in units of* cm^{-1}—Continued

THEORETICAL ASSIGNMENT			J	OBS.	CALC.	O–C	CALC. g
MAIN COMPONENT		ADDITIONAL					
$3d^7(^4F)sp(^3P)\,^2G$			9/2	98276.70	98301	−24	1.115
			7/2	99844.13	99857	−13	.908
$3d^7(^4P)sp(^3P)\,^6S$			5/2		98759		1.997
$3d^7(^4F)sp(^3P)\,^2F$			7/2	99418.61	99222	196	1.130
			5/2	100609.01	100430	179	.876
$3d^7(^4F)sp(^3P)\,^2D$			5/2	101754.80	101718	37	1.186
			3/2	102742.74	102733	10	.803
$3d^8(^3F)5p\,^4D$			7/2	103653.03	103741	−88	1.414
			5/2	104503.22	104590	−87	1.310
			3/2	105439.85	105478	−38	1.125
			1/2	106022.79	106086	−63	.013
$3d^8(^1S)4p\,^2P$			1/2		103459		.667
			3/2		104087		1.329
$3d^8(^3F)5p\,^4G$			11/2	104147.29	104066	81	1.273
	41%	38% ^2G	9/2	105588.89	105496	93	1.164
	55%	24% ^2G	7/2	105499.05	105429	70	1.006
			5/2	106283.16	106228	55	.701
$3d^8(^3F)5p\,^2G$	60%	32% ^4G	9/2	104081.04	104045	36	1.181
	58%	24% ^4G	7/2	106620.53	106525	96	.964
$3d^8(^3F)5p\,^4F$			9/2	104298.23	104285	13	1.271
	39%	33% ^2F	7/2	104646.52	104646	1	1.157
	53%	24% ^4G	5/2	105668.78	105673	− 4	.931
			3/2	106369.30	106399	−30	.463
$3d^8(^3F)5p\,^2D$			5/2	105861.19	106017	−156	1.178
			3/2	107142.12	107313	−171	.822
$3d^8(^3F)5p\,^2F$	46%	32% ^4F	7/2	105838.06	105825	13	1.144
			5/2	107082.21	107080	2	.913
$3d^7(^4P)\,sp\,(^3P)\,^6D$			9/2	105981.50	105888	93	1.554
			7/2		105817		1.585
			5/2		105863		1.654
			3/2		105971		1.837
			1/2		106106		3.296
$3d^7(^4P)\,sp\,(^3P)\,^4S$			3/2	107737.81	107835	−97	1.851
$3d^7(^4P)\,sp\,(^3P)\,^6P$			7/2		108783		1.705
			5/2		108873		1.869
			3/2	109038.84	108901	138	.982
$3d^7(^2G)\,sp\,(^3P)\,^4F$			9/2	109148.05	109136	12	1.324
			7/2	109846.00	109892	−46	1.163
			5/2	110573.36	110573	0	1.022
			3/2	111120.54	111068	53	.518
$3d^7(^2G)\,sp\,(^3P)\,^4H$			13/2		109796		1.228
			11/2		109673		1.135
			9/2		109780		.977
			7/2		110088		.744
$3d^7(^2P)\,sp\,(^3P)\,^4P$			1/2		111112		2.458
	44%	30% ^4D	3/2		111724		1.519
	48%	30% ^4D	5/2		111917		1.506
$3d^7(^2G)\,sp\,(^3P)\,^4G$			11/2		111634		1.263
			9/2		111850		1.160
			7/2	111783.79	112087	−303	.975
			5/2		112329		.584

TABLE 2. Ni II – *Observed and calculated energy levels* $3d^84p+3d^85p+3d^74s4p$ *in units of* cm^{-1} – Continued

THEORETICAL ASSIGNMENT			*J*	OBS.	CALC.	O–C	CALC. *g*
MAIN COMPONENT		ADDITIONAL					
$3d^7(^4P)\,sp\,(^3P)\,^4D$			7/2		111437		1.427
	56%	25% ^4P	5/2		111233		1.437
	44%	24% ^4P	3/2		111271		1.258
			1/2		111497		.166
$3d^7(^4F)\,sp\,(^1P)\,^4G$			11/2	112422.19	112549	−127	1.272
	67%	28% ^4F	9/2	113753.04	113728	25	1.214
	41%	44% ^4F	7/2		114531		1.124
	50%	28% ^2F	5/2	115108.09	115173	−65	.820
$d^7sp\,^4D$			7/2		112683		1.421
			5/2		113262		1.380
	65%	24% ^4P	3/2		113846		1.309
	65%	28% ^4P	1/2		114523		.843
$3d^7(^2G)\,sp\,(^3P)\,^2H$			9/2		113082		.904
			11/2		113952		1.085
$3d^7(^4F)\,sp\,(^1P)\,^4F$	63%	34% ^4G	9/2	113321.95	112935	387	1.275
	28%	29% ^4G + 29% ^2G	7/2	114052.21	113788	264	1.056
	61%	16% ^2F	5/2	115120.00	114836	284	1.046
	60%		3/2		115149		.761
$3d^7(^2G)\,sp\,(^3P)\,^2G$	58%	25% ^4G + 14% ^4F	7/2		113765		.970
			9/2		114276		1.119
$3d^7(^4P)\,sp\,(^3P)\,^2S$			1/2		113841		1.925
$3d^7(^4P)\,sp\,(^3P)\,^4P$	61%		5/2		114043		1.456
	53%	40% ^4D	3/2		114387		1.495
	38%	40% ^4D + 20% ^2S	1/2		114378		1.459
$3d^7(^2G)\,sp\,(^3P)\,^2F$	29%	46% ^4G	5/2		114229		.831
	51%	22% ^4D	7/2	115000.25	114866	134	1.209
$3d^7(^2H)\,sp\,(^3P)\,^4G$			11/2	114858.88	114996	−137	1.269
			9/2	116087.38	115720	367	1.139
			7/2	116275.81	116379	−103	1.019
			5/2	116824.15	116833	−9	.643
$d^7sp\;\,^2D$	62%		3/2	114869.35	115018	−149	.923
	50%	33% ^4D	5/2	116893.98	117046	−152	1.237
$d^7sp\;\,^4D$	78%		1/2		115177		.461
	30%	42% ^4F	3/2	115592.25	115568	24	.834
	32%	25% ^4F + 23% ^2D	5/2	115565.98	115340	226	1.154
	55%	18% ^2F	7/2	115209.98	115321	−111	1.298
$3d^7(^2H)\,sp\,(^3P)\,^4I$			15/2		115245		1.200
			13/2		115237		1.109
			11/2		115440		.977
			9/2		115784		.785
$3d^7(^4P)\,sp\,(^3P)\,^2D$	61%	27% ^4D	5/2		115868		1.245
	43%	25% ^2P	3/2		117094		1.057
$d^7sp\;\,^4D$			7/2	116512.06	116603	−91	1.408
	50%	23% ^4F	5/2		117595		1.242
	40%	23% ^4S + 21% ^2P	3/2		117989		1.384
	38%	26% ^2P + 23% ^2S	1/2		118159		.758
$3d^7(^2P)\,sp\,(^3P)\,^4S$	37%	12% ^2D + 12% ^4F	3/2	117662.11	117460	202	1.417
$d^7sp\;\,^2P$	41%	23% ^2S	1/2		117478		.984
	27%	29% ^4D + 21% ^4F	3/2		118284		1.118
$3d^7(a\,^2D)\,sp\,(^3P)\,^4F$			9/2	117593.68	117552	42	1.333
			7/2	117972.47	117993	−21	1.250
	48%	24% ^2D	5/2		118627		1.094
	32%	32% ^2D + 17% ^2P	3/2		118786		.874

TABLE 2. Ni II—*Observed and calculated energy levels* $3d^84p+3d^85p+3d^74s4p$ *in units of* cm^{-1}—Continued

THEORETICAL ASSIGNMENT							
MAIN COMPONENT		ADDITIONAL	J	OBS.	CALC.	O–C	CALC. g
$3d^8(^1D)5p\ ^2D$	36%	$12\%(^1D)^2P$	3/2	117763.91	117858	−94	1.165
	65%		5/2	117872.78	117995	−122	1.271
$3d^7(^2H)\,sp\,(^3P)^2I$			11/2	118248.98	118305	−56	.928
			13/2	119010.21	118992	18	1.085
$3d^8(^1D)5p\ ^2F$			5/2	118379.11	118389	−10	.979
			7/2	118563.39	118542	21	1.193
$3d^8(^1D)5p\ ^2P$	37%	$35\%(^1D)^2D$	3/2	118442.81	118510	−67	1.158
	50%	$29\%d^7\,sp\,^4D$	1/2	118631.95	118503	128	.606
$3d^7(^2P)\,sp\,(^3P)\ ^2S$	36%	$44\%^2P$	1/2		119423		1.438
$3d^7(^2H)\,sp\,(^3P)\ ^4H$			13/2		119729		1.226
			11/2		120027		1.133
			9/2		120280		.976
			7/2		120498		.692
$3d^8(^3P)5p\ ^4P$	51%	$19\%(^1D)^2D$	5/2	119796.98	119905	−108	1.518
	36%	$17\%(^1D)^2P$	3/2	120166.52	120221	−54	1.534
			1/2	120316.02	120260	56	2.406
$3d^7(^2P)sp(^3P)\ ^2P$	54%		1/2		119906		.679
	31%	$36\%d^85p\,^4P$	3/2		119945		1.385
$3d^7(a^2D)sp(^3P)\ ^4P$			5/2		120612		1.527
	44%	$17\%^2P$	3/2		121766		1.535
			1/2		122378		2.393
$3d^8(^3P)5p\ ^4D$	81%		7/2	120903.31	121052	−149	1.387
	63%	$27\%(^3P)^2D$	5/2	121325.09	121302	23	1.322
	54%		3/2	121385.80	121307	79	1.227
	83%		1/2	121561.06	121445	116	.064
$3d^8(^3P)5p\ ^2P$	35%	$18\%^2D+17\%^2S$	3/2	121042.57	121091	−48	1.260
			1/2		121917		.751
$3d^8(^3P)5p\ ^2D$	57%	$20\%(^3P)^4D$	5/2	121050.66	121007	44	1.216
	28%	$32\%(^3P)^2P$	3/2	121800.34	121662	138	1.260
$3d^8(^3P)5p\ ^4S$	43%	$23\%(^3P)^2D$	3/2	121456.30	121409	47	1.509
$3d^7(^2H)sp(^3P)\ ^2G$			9/2	121692.55	121749	−56	1.108
			7/2	121862.57	121882	−19	.873
$3d^7(a^2D)sp(^3P)\ ^2F$			5/2		121963		.914
			7/2		122670		1.150
$3d^8(^3P)5p\ ^2S$			1/2		122063		1.883
$3d^7(a^2D)sp(^3P)\ ^2D$			3/2		122131		.930
			5/2		122277		1.204
$3d^7(a^2D)sp(^3P)\ ^2P$			1/2		124474		.751
			3/2		124771		1.362
$3d^7(^2H)sp(^3P)\ ^2H$			9/2	124652.00	124787	−135	.911
			11/2	125003.41	125159	−156	1.092
$3d^8(^1G)5p\ ^2F$			7/2	127219.57	126938	282	1.142
			5/2	127331.60	127071	261	.858
$3d^8(^1G)5p\ ^2H$			9/2	126679.98	126895	−215	.910
			11/2	126857.97	127061	−203	1.091

453-425 OL - 72 - 5

TABLE 2. Ni II — *Observed and calculated energy levels* 3d⁸4p + 3d⁸5p + 3d⁷4s4p *in units of cm⁻¹* — Continued

THEORETICAL ASSIGNMENT						
MAIN COMPONENT	ADDITIONAL	J	OBS.	CALC.	O–C	CALC. g
$3d^7(^4P)sp(^1P)\ ^4S$		3/2	126738.82	126903	−164	1.990
$3d^8(^1G)5p\ ^2G$		9/2	127885.86	127896	−10	1.110
		7/2	127895.33	127888	7	.890
$3d^7(^4P)sp(^1P)\ ^4D$		7/2	129782.07	129925	−143	1.427
		5/2	129988.05	130121	−133	1.366
		3/2	130331.78	130372	−40	1.200
		1/2	130570.42	130595	−25	.037
$3d^7(^2G)sp(^1P)\ ^2H$		11/2	131424.32	131131	293	1.086
		9/2	132311.98	132116	196	.915
$3d^7(^2F)sp(^3P)\ ^4G$		5/2		132462		.611
		7/2		132685		1.012
		9/2		133035		1.188
		11/2	133625.96	133567	59	1.272
$3d^7(^4P)sp(^1P)\ ^4P$		5/2	(131834.94)	132957	(−1122)	1.548
		3/2	(132225.15)	133323	(−1098)	1.681
		1/2	(132120.70)	133328	(−1208)	2.490
$3d^7(^2G)sp(^1P)\ ^2F$		7/2	133169.92	132917	253	1.138
		5/2	134208.30	134110	98	.994
$3d^7(^2F)sp(^3P)\ ^4F$		3/2	133190.19	132894	296	.425
		5/2	133209.30	133179	30	1.021
		7/2	133528.02	133541	−13	1.214
		9/2	133853.04	133898	−45	1.303
$3d^7(^2G)sp(^1P)\ ^2G$		9/2	133445.75	133676	−230	1.116
		7/2	134380.82	134783	−402	.891
$3d^7(^2F)sp(^3P)\ ^4D$		7/2	133850.83	133888	−37	1.417
		5/2	133973.33	133885	87	1.225
		3/2	134156.28	134113	43	1.198
		1/2	134283.76	134215	69	.047
$3d^7(^2F)sp(^3P)\ ^2D$		5/2	134783.14	134841	−58	1.205
		3/2	134964.78	135024	−59	.913
$3d^7(^2P)sp(^1P)\ ^2P$		1/2		135549		.776
		3/2	135382.53	135661	−278	1.169
$3d^7(^2F)sp(^3P)\ ^2G$		7/2	135746.06	135737	9	.894
		9/2	136076.26	135942	134	1.112
$3d^7(^2P)sp(^1P)\ ^2D$		5/2	(135258.92)	135900	(−741)	1.200
		3/2		137089		.826
$3d^7(^2H)sp(^1P)\ ^2I$		13/2		136509		1.077
		11/2		137494		.929
$3d^7(a^2D)sp(^1P)\ ^2D$		5/2		138244		1.154
		3/2		139402		.864
$3d^7(^2H)sp(^1P)\ ^2G$		9/2	138495.84	138613	−117	1.109
		7/2		139322		.906
$3d^7(^2F)sp(^3P)\ ^2F$		7/2		138858		1.138
		5/2		139447		.889
$3d^7(^2P)sp(^1P)\ ^2S$		1/2		139683		1.911
$3d^7(a^2D)sp(^1P)\ ^2F$		7/2		139904		1.140
		5/2		141012		.902
$3d^7(^2H)sp(^1P)\ ^2H$		11/2		141873		1.091
		9/2		142868		.913

TABLE 2. Ni II—*Observed and calculated energy levels* $3d^84p+3d^85p+3d^74s4p$ *in units of* cm^{-1}—Continued

THEORETICAL ASSIGNMENT		J	OBS.	CALC.	O–C	CALC. g
MAIN COMPONENT	ADDITIONAL					
$3d^7(a^2D)sp(^1P)\ ^2P$		3/2		142107		1.332
		1/2		143961		.738
$3d^7(b^2D)sp(^3P)\ ^4P$		5/2		151277		1.598
		3/2		151257		1.730
		1/2		151281		2.661
$3d^7(b^2D)sp(^3P)\ ^4F$		3/2		152576		.403
		5/2		152859		1.029
		7/2		153254		1.237
		9/2		153760		1.330
$3d^8(^1S)5p\ ^2P$		1/2		153513		.667
		3/2		154114		1.148
$3d^7(^2F)sp\ (^1P)\ ^2G$		7/2		154379		.890
		9/2		154810		1.114
$3d^7(^2F)sp\ (^1P)\ ^2D$		3/2		154619		.986
		5/2		154998		1.078
$3d^7(^2F)sp\ (^1P)\ ^2F$		5/2		155556		.979
		7/2		155892		1.143
$3d^7(b^2D)\ sp\ (^3P)\ ^2P$		3/2		156895		1.330
		1/2		157329		.623
$3d^7(b^2D)\ sp\ (^3P)\ ^2F$		5/2		157904		.869
		7/2		158157		1.166
$3d^7(b^2D)\ sp\ (^3P)\ ^4D$		1/2		158243		.048
		3/2		158398		1.200
		5/2		158717		1.359
		7/2		159298		1.405
$3d^7(b^2D)\ sp\ (^3P)\ ^2D$		5/2		161296		1.200
		3/2		161382		.803
$3d^7(b^2D)\ sp\ (^1P)\ ^2P$		1/2		173566		.667
		3/2		174048		1.332
$3d^7(b^2D)\ sp\ (^1P)\ ^2F$		5/2		174919		.858
		7/2		175397		1.142
$3d^7(b^2D)\ sp\ (^1P)\ ^2D$		3/2		179748		.800
		5/2		180530		1.199

of the $d-f$ interaction and for ζ_f was done by direct observation of the experimental level values. The final parameters which we obtained for these configurations are given in table 3. In column L.S.a, all the parameters were set free, and the rms error is 25.6 cm^{-1}. We can see that the parameters $F_4(df)$, $G_3(df)$ and ζ_f are equal to zero within their statistical accuracy. Column L.S.b of table 3 gives the results of a calculation in which the above-mentioned parameters were fixed at zero. In this case the rms error is 25.2 cm^{-1}. The observed and calculated levels of d^8f are given in table 4.

We would like to emphasize that the d^8f configuration was calculated independently without including any interaction with any other configuration. This simple treatment is justified to some extent by the small mean error.

In all, 60 experimental levels of d^8f were fitted to the calculated ones. Three observed levels could not be fitted. They are:

$$132729.48\ cm^{-1}\ \text{with}\ J=5/2,$$

$$135954.09\ cm^{-1}\ \text{with}\ J=7/2,$$

$$135580.25\ cm^{-1}\ \text{with}\ J=9/2.$$

TABLE 3. *Parameters of the Configuration* d⁸f

All values are in units of cm^{-1}

P	Diag.	L.S.a	L.S.B
$A-3d^84f$	128190	128189. ±	128186 ±5
B	1035	1035.4±0.6	1035.5±0.6
C	4080	4086 ±6	4086 ±6
$F_2(df)$	8.5	8.4±0.5	8.3±0.4
$F_4(df)$	0	0.1±0.1	....
$G_1(df)$	1	1.6±0.8	1.4±0.6
$G_3(df)$	0	0.3±0.3	....
$G_5(df)$	0	0.03±0.05	....
ζ_d	670	668 ±3	668 ±3
ζ_f	0	3 ±2	....
Δ	....	25.6 cm^{-1}	25.2 cm^{-1}

The coupling for this configuration is the $J-l$ coupling; that is: the S' and L' of the d^8 parent term first combine to form J''. Then J'' is combined with the $l=3$ of the f electron forming K and finally the spin of this electron is added to K and the total J is formed. This is the coupling used in table 4.

The authors wish to express their deep gratitude to Professor Shenstone for the special pleasure and benefit of his kind and useful cooperation.

TABLE 4. *Ni* II—*Observed and calculated energy levels* 3d⁸4f

THEORETICAL ASSIGNMENT		J	OBS.	CALC.	O–C	CALC. g
d^8 PARENT	K					
$^3F_4$	7	13/2	118803.82	118837	−33	1.086
		15/2	118848.92	118837	12	1.200
	1	3/2	118809.34	118800	9	1.779
		1/2	118774.76	118805	−30	1.523
	2	5/2	118828.61	118833	−4	1.448
		3/2	118877.09	118853	24	1.143
	3	7/2	118874.11	118871	3	1.329
		5/2	118897.94	118900	−2	1.094
	6	11/2	118892.99	118909	−16	1.081
		13/2	118893.24	118909	−16	1.212
	4	9/2	118914.34	118905	9	1.269
		7/2	118923.20	118924	−1	1.082
	5	9/2	118927.02	118924	3	1.081
		11/2	118939.53	118924	16	1.234
$^3F_3$	0	1/2	120189.55	120170	20	2.043
	1	3/2	120199.18	120194	5	1.379
		1/2	120203.49	120181	22	.704
	2	5/2	120203.49	120222	−19	1.244
		3/2	120222.89	120224	−1	.861
	6	11/2	120211.30	120205	6	.970
		13/2	120218.22	120205	13	1.117
$^3F_3$	3	7/2	120250.17	120249	1	1.176
		5/2	120271.97	120265	7	.909
	4	7/2	120268.81	120281	−12	.938
		9/2	120281.11	120272	9	1.146
	5	11/2	120270.44	120265	5	1.124
		9/2	120272.53	120265	8	.949
$^3F_3$	1	3/2	121042.52	120092	−49	1.540
		1/2	121090.71	121092	−1	1.059
	5	11/2	121120.88	121122	−1	.976
		9/2	121125.41	121122	3	.771
	2	5/2	121146.98	121146	1	1.181
		3/2	121161.81	121147	15	.763

TABLE 4. *Ni* II—*Observed and calculated energy levels* 3d⁸4f—Continued

THEORETICAL ASSIGNMENT		J	OBS.	CALC.	O–C	CALC. g
d^8 PARENT	K					
	4	7/2	121178.56	121192	−13	.762
		9/2	121180.54	121190	−9	1.008
	3	7/2	121192.32	121183	9	1.063
		5/2	121194.14	121188	6	.753
$^1D_2$	4	9/2	132818.16	132855	−37	1.138
		7/2	132846.53	132857	−10	.933
	3	5/2	(132729.48)	132875	(−146)	.878
		7/2	132869.16	132889	−20	1.148
$^1D_2$	2	5/2	132912.15	132944	−32	1,197
		3/2	132927.97	132940	−12	.793
	1	3/2	132982.51	133005	−23	1.283
		1/2	133001.47	133005	−4	.564
	5	11/2	133014.08	132950	64	1.119
		9/2	133031.00	132950	81	.943
$^3P_2$	3	7/2	135400.67	135438	−37	1.179
		5/2	135461.55	135452	10	.979
	4	9/2	135435.26	135414	21	1.283
		7/2	135444.47	135430	14	1.127
	2	3/2	135493.26	135485	8	.515
		5/2	135512.92	135501	12	.976
	5	11/2	135538.61	135582	−43	1.243
		9/2	135558.80	135582	−23	1.092
	1	3/2	135652.93	135661	−8	1.057
		1/2	135670.49	135659	11	.106
$^3P_1$	2	5/2		135784		1.255
		3/2	135746.13	135784	−38	.885
	4	9/2	(135580.35)	135773	(−193)	1.179
		7/2	(135464.86)	135776	(−311)	.976
	3	5/2	135849.41	135866	−17	.895
		7/2	135879.41	135864	15	1.174
$^3P_0$	3	7/2	(135954.09)	136055	(−101)	1.176
		5/2	136122.61	136056	67	.905
$^1G_4$	1	3/2		140232		1.334
		1/2		140233		.667
	2	5/2		140345		1.200
		3/2		140347		.800
	7	13/2		140355		.933
		15/2		140355		1.067
	3	7/2		140491		1.143
		5/2		140492		.857
	4	9/2		140632		1.111
		7/2		140632		.889
	6	11/2		140643		.923
		13/2		140643		1.077
	5	11/2		140708		1.091
		9/2		140708		.909
$^1S_0$	3	7/2		171363		1.143
		5/2		171364		.857

5. References

[1] Moore, C. E., Atomic Energy Levels, NBS Circ 467, II (1949).
[2] Steinberger, H., Msc. Thesis, The Hebrew University of Jerusalem, 1958.
[3] Shimoni, Z., Msc. Thesis, The Herbrew University of Jerusalem, 1959.
[4] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **73A** (Phys. and Chem.) No. 2, 129, (1969).
[5] Shenstone, A. G., J. Res. Nat. Bur. Stand. (U.S.), **74A** (Phys. and Chem.) No. 6, 801, (1970).
[6] Schwimmer, A., Msc. Thesis, The Hebrew University of Jerusalem (1967).
[7] Racah, G., and Shadmi, Y., Bull. Res. Counc. of Israel **8F,** 15 (1959).
[8] Shadmi, Y., and Caspi, E., Oreg J. Res., Nat. Bur. Stand. (U.S.), **73A** (Phys. and Chem.) No. 2, 173, 1969.
[9] Shadmi, Y., Phys. Rev. **139A,** 43 (1965).
[10] Shadmi, Y., Oreg, J., Stein, J., J.O.S.A. **58,** 7, 909–914 (1968).

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