JOURNAL OF RESEARCH of the National Bureau of Standards—A. Physics and Chemistry
Vol. 74A, No. 5, September–October 1970

Odd Configurations in Neutral Nickel (Ni I)*

Charles Roth**

(May 28, 1970)

Experimental levels of the configurations $3d^94p$, $3d^84s4p$ and $3d^95p$ of Ni I were compared with corresponding calculated values. The electrostatic interactions between the configurations $(3d+4s)^94p$ as well as between $3d^84s4p$ and $3d^95p$ were considered explicitly.

For the configurations $(3d+4s)^94p$, 71 experimental levels were fitted by means of 17 free parameters to yield an rms error of 131 cm^{-1}. On fitting 83 levels of the configurations $3d^94p+3d^84s4p+3d^95p$ by means of 25 free parameters an rms error of 147 cm^{-1} was obtained.

Key words: Energy levels; g-factors; interactions between configurations; nickel; $(3d+4s)^94p$; $3d^94p+3d^84s4p+3d^95p$.

1. The Configurations $(3d+4s)^94p$

The configurations $(d+s)^9p$ comprise 92 terms splitting into 212 levels. In AEL [1][1], 27 terms splitting into 66 levels are assigned to the configurations $3d^94p+3d^84s4p$, and in addition, there are 6 unclassified odd levels. As in Co I [7], only the initial values for the parameters[2] B', C', and α', were obtained by linear extrapolation from the results of Sc I–Co I [2–7]. Then,

$$\begin{aligned} B' &= 1040 \\ C' &= 4140 \\ \alpha' &= \ \ 84 \end{aligned} \tag{1}$$

The initial values of the other parameters were taken as the final values of Co I [7].

The initial value for the height of the configuration $3d^84s4p$ can be obtained either from the electrostatic matrices of ^5F or ^5G (they only differ by $4F_2'$). Then from ^5G, we have [1], [8]

$$^5G_{C.G.} = A' - 8B' - 2G_{ds}' - F_2' - G_{ps}' + 12\alpha' = 27900 \tag{2}$$

Hence, from the values of the previously determined parameters

$$A' = 45670 \tag{3}$$

The height of the configuration $3d^94p$ was obtained from the electrostatic matrix of $3d^94p\,^3P$, since the terms ^3P of $3d^84s4p$ are sufficiently high that the interaction with them is not strong.

Then, since

$$3d^94pz\,^3P_{C.G.} = A - 7F_2 = 29330 \tag{4}$$

initially,

$$A = 30870 \tag{5}$$

It should be noted that the above value of A contains the contribution 6α, since the constant matrix of α for d^9p was not put on tape.

The parabola used to find D″ (Co I) [7], extrapolated further gives

$$D''[\text{Ni I}] = 48300 \tag{6}$$

By using the values of B'' and C'' from V I to Co I [3–7] in order to obtain the best straight lines for these parameters, and extrapolating to Ni I

$$\begin{aligned} B'' &= 1190 \\ C'' &= 4190 \end{aligned} \tag{7}$$

Then, from eqs (8) and (9), [5]

$$A'' = 85680 \tag{8}$$

The final values of the parameters obtained in the uniform treatment[3] are given in table 1.

The final value of A'' was fixed at 85060, so that with the new values of the parameters, D'' (Ni I) should approximately equal the original value of 48300.

*An invited paper.

**Present address: Department of Mathematics, McGill University, Montreal 110, Canada.

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

[2] Unprimed parameters refer to the configuration $3d^94p$, primed parameters to $3d^84s4p$, and doubly primed to $3d^74s^24p$.

The numerical values of all levels and parameters are in cm^{-1}.

[3] The parameters A, A', G_{ds}', and G_{ps}' are allowed to change freely. The parameters B, C, F_2, and G_1 are in arithmetic progression. The parameters G_3, α, ζ_d, and ζ_p are kept equal, and for the parameters of the interactions between configurations H' is kept equal to H, J' to J, G to G_{ds}' and $K'=K+956$ (fixed difference).

From the values of B', B'', C', and C'' obtained for first spectra investigated previously it was apparent that the approximate differences were:

$$\begin{aligned} B''-B' &= 85 \\ C''-C' &= 100 \end{aligned} \tag{9}$$

These differences were kept fixed in the least-squares calculations.

In order to estimate the effects of the interactions with the configurations $3d^74s^24p$, the configurations $3d^94p+3d^84s4p$ were also considered without $3d^74s^24p$. Although $3d^74s^24p$ is very high, the rms error rose from the present value of 131 to 173, stressing the importance of inserting the interactions with $3d^74s^24p$ explicitly. Although all the levels had higher deviations without $3d^74s^24p$, the level $^3F(^1P)y\,^3G_5$ [4] can be singled out in particular. Whereas in the case of $(3d+4s)^94p$ the deviation for this level was 330, for $3d^94p+3d^84s4p$ the deviation rose to 540. The final parameters for $3d^94p+3d^84s4p$ are given in table 1.

Since it was not possible to perform a variation in the least-squares with A'' free, the calculated values of the levels $3d^74s^24p$ are not significant. The comparison of the experimental and calculated values of the levels and the g-factors of the configurations $3d^84p+3d^74s4p$ are given in table A of the appendix, when these configurations were considered together with $3d^95p$.

2. Ni I $-3d^94p+3d^84s4p+3d^95p$

All the predicted levels of the configuration $3d^95p$ have been observed experimentally. Furthermore, since the configuration $3d^95p$ lies in the middle of the range of observed levels of $3d^84s4p$, it is interesting to investigate the effect of the interaction between $3d^84s4p$ and $3d^95p$. The necessary matrices comprising the configurations d^9p, d^8sp, d^9p' and the interactions d^9p-d^8sp and $d^9p'-d^8sp$ had already been lculated for Cu II [9].

The initial values for the parameters of $3d^94p+3d^84s4p$ were taken as the final values obtained for Ni I $(3d+4s)^94p$.

For $3d^95p$, the initial values of A^*[5] and F_2^* were obtained from the electrostatic matrices of ^3P, ^3D, and ^3F. By using the centers of gravity of the three terms and least-squares to reduce the 3 equations in 2 unknowns to 2 equations in 2 unknowns the solution gives

$$\begin{aligned} A^* &= 49260 \\ F_2^* &= \quad 37 \end{aligned} \tag{10}$$

Since the matrices of J equal to 0 and 4 are of order 1, we obtain from $^3P_0$, $^3F_4$, and (10) initially

$$\begin{aligned} \zeta_d^* &= 640 \\ \zeta_p^* &= 340 \end{aligned} \tag{11}$$

Then, by using the fact that the trace equals the sum of the eigenvalues we obtain from the matrices of J equal to 1 and 3:

$$\begin{aligned} G_1^* &= 95 \\ G_3^* &= 13 \end{aligned} \tag{12}$$

The above initial values were used at first in the diagonalization of $3d^95p$ alone. After two iterations the following values were obtained:

$$\begin{aligned} A^* &= 49470 \pm 43 \\ F_2^* &= \quad 42 \pm 9 \\ G_1^* &= \quad 73 \pm 10 \\ G_3^* &= \quad 0 \text{ (Fixed)} \\ \zeta_d^* &= 531 \pm 36 \\ \zeta_p^* &= 159 \pm 82 \\ \text{rms error} &= 139.4 \text{ cm}^{-1} \end{aligned} \tag{13}$$

The parameter G_3^* was eliminated, since it had a value of -9 ± 9 when left to change freely.

Guided partly by the results of Cu II [9], the initial values for the parameters J^* $(3d^95p-3d^84s4p)$ and K^* $(3d^95p-3d^84s4p)$ were taken to equal about half of the corresponding values of J and K. Then, from table 1

$$\begin{aligned} J^* &= 500 \\ K^* &= 1000 \end{aligned} \tag{14}$$

In the final variation of the least-squares all the 33 terms splitting into 78 levels, which are assigned to $3d^94p+3d^84s4p+3d^95p$ in AEL, were inserted. In addition, 5 unclassified levels were also included. The values of the parameters for the three configurations are given in table 1.

The parameter F_2^* was eliminated since it assumed a small negative value when left to change freely.

The values for the parameters G_3, G_3^*, and ζ_p^* are not meaningful since the standard errors are larger than the numerical values of the parameters.

The values for the parameters J^* and K^* are important since they provide the only information about the strength of the interaction $3d^n5p+3d^{n-1}4s4p$ in the first spectra of the iron group.

The calculated values, percentages compositions and g-factors of all the 114 predicted levels (50 terms) of $3d^94p+3d^84s4p+3d^95p$ are given in table A (appendix).

The only odd level not included was 3° at 44336.10. An examination of the combinations of the level 3° as given by Russell [10], reveals that this level is based upon combinations with only the two even levels $a\,^3F_3$ and $a\,^3F_4$. From table A it is evident that this level could conceivably be assigned to $^3P(^3P)^5D_4$, yielding a deviation of around 300. However, since it is doubtful whether 3° is a valid level, this assignment was rejected.

[4] For the theoretical term designations see the appendix of this paper.

[5] Starred parameters refer to the configuration $3d^95p$.

TABLE 1. *Final parameters in units of* cm^{-1}

Parameter	$(3d+4s)^9 4p$	$3d^9 4p + 3d^8 4s 4p$	$3d^9 4p + 3d^8 4s 4p + 3d^9 5p$
A	31158 ± 156	30814 ± 218	31016 ± 161
A'	45786 ± 139	45144 ± 167	45352 ± 140
A''	85060 (Fixed)	.....	.....
A^*	.....	.....	49417 ± 183
B'	1024 ± 7	1017 ± 10	1011 ± 9
B''	1109 (Fixed)	.....	.....
C'	4187 ± 54	4202 ± 73	4112 ± 66
C''	4287 (Fixed)	.....	.....
F_2	166 ± 13	148 ± 18	159 ± 15
F_2'	311 ± 7	304 ± 9	315 ± 8
F_2''	456 (Arith. Progress.)	.....	.....
F_2^*	.....	.....	0 (Fixed)
G_1''	165 ± 9	166 ± 13	163 ± 12
G_1	223 ± 9	240 ± 14	251 ± 13
G_1'	281 (Arith. Progress.)	.....	.....
G_1^*	.....	.....	41 ± 14
$G_3 = G_3'$	14 ± 4	15 ± 5	15 ± 6
$G_3'' = G_3'$	14 (Equal)	.....	.....
G_3^*	.....	.....	3 ± 10
G_{ds}'	1626 ± 53	1505 ± 90	1470 ± 81
$G = G_{ds}'$	1626 (Equal)	.....	.....
G_{ps}'	7027 ± 60	6705 ± 67	6755 ± 55
α'	83 ± 7	81 ± 11	59 ± 11
$\alpha'' = \alpha'$	83 (Equal)	.....	.....
H	154 ± 33	159 ± 64	174 ± 48
$H' = H$	154 (Equal)	.....	.....
J	1144 ± 34	693 ± 219	1003 ± 155
$J' = J$	1144 (Equal)	.....	.....
$J^*(3d^9 5p - 3d^8 4s 4p)$	.....	.....	573 ± 77
K	2072 ± 135	1691 ± 223	2010 ± 162
K'	3028 (Fixed Diff.)	.....	.....
$K^*(3d^9 5p - 3d^8 4s 4p)$	.....	.....	996 ± 74
ζ_d: ζ_d'	603 ± 19	581 ± 26	600 ± 22
$\zeta_d'' = \zeta_d'$	603 (Equal)	.....	.....
ζ_d^*	.....	.....	596 ± 51
$\zeta_p = \zeta_p'$	255 ± 51	229 ± 62	206 ± 59
$\zeta_p'' = \zeta_p'$	255 (Equal)	.....	.....
ζ_p^*	.....	.....	51 ± 120
rms error	131.1 cm^{-1}	173.3 cm^{-1}	147.0 cm^{-1}

There were the following changes in assignment:

1. AEL $3d^8 4s(b\,^2D)4py\,^3P_{1,2}$ ⟶ $^1D(^3P)^3D_{1,2}$
2. AEL $3d^8 4s(b\,^2D)4px\,^3D_2$ ⟶ $^1D(^3P)^3F_2$
3. $^3F(^1P)^3D_3$ ⟷ $^1D(^3P)^3F_3$
4. AEL $3d^8 4s(b\,^2D)4py\,^1P$ ⟶ $^1D(^3P)^3P_1$
5. AEL $3d^8 4s(b\,^2D)4px\,^1D$ ⟶ $^1D(^3P)^3P_2$
6. AEL $3d^8 4s(b\,^2D)4px\,^1F$ ⟶ $^3P(^3P)^5D_3$
7. $^3F(^1P)^3F_3$ ⟷ $^3F(^1P)^3G_3$
8. $5p\,^1F$ ⟷ $5p\,^3F_3$
9. $5p\,^3D_2$ ⟷ $5p\,^1D$

The calculated values of the levels $^1D(^3P)^3P_{1,2}$ are, on the average, higher by 1000 than the experimental values of the levels $y\,^3P_{1,2}$. Such high deviations would be completely inconsistent with all the results obtained thus far. However, the experimental levels $y\,^3P_{1,2}$ correspond very closely to the calculated values of the levels $^1D(^3P)^3D_{1,2}$ but there is a very large discrepancy between the experimental g-factor of 1.32 for $y\,^3P_1$ and the calculated g-factor of 0.643 for $^1D(^3P)^3D_1$.

Experimental g-factors for Ni I were obtained by Bakker [11], Marvin and Baragar [12], Dijkstra [13], and Lindsley [14]. For many levels 4 different g-factors were obtained, usually differing from each other by very little. However, the experimental g-factor for $y\,^3P_1$ was obtained only by Lindsley [14]. Furthermore, not only is the value of 1.32 based on one very weak separate line, $b\,^3D_2 - y\,^3P_1$, with only one measurement used to determine this value, but, actually "only the difference of the g's could be determined from the pattern because of overlapping", [14]. Then the average

389-821 O - 70 - 8

g-factor of the better known level, here $b\,^3D_2$, was assumed.

Thus, we felt justified in neglecting the g-factor of 1.32 and performing the first change above, yielding deviations of only 37 and 64.

The experimental level $x\,^3D_2$ at 42954 is then assigned to the previously vacant theoretical level $^1D(^3P)^3F_2$, yielding a deviation of only -22. The experimental g-factor of 0.840 corresponds to the calculated value of 0.744.

The experimental level $x\,^3F_4$ fits very well in height and g-factor to the corresponding calculated values of $^1D(^3P)^3F_4$. However, the experimental level $x\,^3F_3$, whose term designation is questioned by Russell [10], (the question mark is not in the right place in AEL), cannot be assigned to $^1D(^3P)^3F_3$, as the deviation would then be about 900, which is completely incompatible with the deviations of -22 and -10 obtained for the other two levels assigned to $^1D(^3P)^3F$. Thus, as indicated by change 3, the level $w\,^3D_3$ is assigned to $^1D(^3P)^3F_3$ with a resulting deviation of only -54 and excellent agreement between the experimental and calculated g-factors (1.22 vs 1.189). Then the experimental level $x\,^3F_3$ is assigned to the vacant level $^3F(^1P)^3D_3$, yielding a deviation of only -119. The experimental g-factor of 1.24 compares favorably with the calculated value of 1.317.

The calculated values of the terms $^1D(^1P)^1D$ and $^1D(^1P)^1P$ are 58144 and 58832, respectively. Thus, the experimental terms $x\,^1D$ and $y\,^1P$ cannot be fitted to the theoretical terms with the same designations. As indicated by the changes 4 and 5, these two levels are assigned to the vacant levels $^1D(^3P)^3P_{1,2}$ (see change 1). The resulting deviations are only 18 and 0, and there is excellent agreement between the experimental and calculated g-factors (the experimental values of 1.48 and 1.39 correspond to the calculated values of 1.457 and 1.418, respectively).

Similarly, since the calculated value of the term $^1D(^1P)^1F$ is 56358 the experimental term $x\,^1F$ is erroneously designated. Russell, [10], observed that $x\,^1F$ has combinations with the levels of $a\,^3D$, $a\,^3F$ and $a\,^1D$. However, the transition with $a\,^1D$ is questioned and thus, we felt justified in assigning $x\,^1F$ to the only vacant theoretical level with J-value of 3 in that range, i.e., $^3P(^3P)^5D_3$, as indicated by change 6. The resulting deviation is only 47.

When the levels $w\,^3F_3$ and $y\,^3G_3$ were assigned to the theoretical levels with the same term designations, the deviations were -562 and 714, respectively. When these two levels are interchanged the deviations for $w\,^3F_3$ and $y\,^3G_3$ are only -19 and 154, respectively. However, then the experimental values of 0.78 and 1.04 for the g-factors do not agree well with the calculated values of 1.059 and 0.784, respectively. As in the case of $y\,^3P_1$, of the 4 sources of the experimental g-factors of Ni I, the values for $w\,^3F_3$ and $y\,^3G_3$ were obtained only by Lindsley, [14]. The g-factor of 1.04 is based on two lines, one of which is unresolved, and the g-factor of 0.78 is based on only one unresolved line. In *all* cases, the average g-factors for the even levels ($a\,^3F_2$ and $a\,^3F_3$) were *assumed* in order to obtain the g-factor for the odd levels. Thus, as for $y\,^3P_1$, the discrepancies in the g-factors were disregarded, and the exchange 7 performed.

For the exchange 8 it should be noted that the eigenfunctions of $5p\,^1F$ and $5p\,^3F_3$ are mixed strongly. In the configuration $3d^95p$ the coupling is more likely Jl than LS which explains the large mixture of LS components.

The last exchange had already been performed when the configuration $3d^95p$ was considered alone. Since the calculated values of the levels $5p\,^1D$ and $5p\,^3D_2$ are 49003 and 50674, respectively, it is evident that the term designations for the two experimental levels $5p\,^3D_2$ at 49185 and $5p\,^1D$ at 50689 should be interchanged.

The eigenfunctions of the levels $^3F(^3P)y^3D_2$ and $^3F(^3P)y\,^3F_2$ are so strongly mixed that it is not meaningful to give one particular term designation to each level.

It should be emphasized that as in previous configurations investigated the parameters were first determined—within small ranges of possible fluctuations—by those levels inserted whose experimental and theoretical term designations coincided. The other levels, with changed assignments, were only inserted later.

The following table gives the assignments of the undesignated levels:

TABLE 2. *Undesignated odd levels of* Ni I

Level	Assignment	Deviation	Obs. g-factor	Calc. g-factor
1°_3	$^3P(^3P)^5P_3$	74	.....	1.633
2°_2	$^3P(^3P)^5P_2$	26	.....	1.796
3°	$(^3P(^3P)^5D_4)$	(336)	.....	(1.294)
4°_2	$^3P(^3P)^5S_2$	-188	.....	1.874
$5^\circ_{2,1}$	$^3P(^3P)^1P_1$	91	.....	1.063
6°_3	$^3P(^3P)^1D_2$	-104	.....	1.030

As explained before, the level 3° was not included in the least-squares, and thus entries pertaining to it are given in parentheses.

For the level 6°, Russell [10], gives 7 combinations with the levels of the 4 even terms $a\,^3P$, $a\,^1D$, $a\,^3F$, and $a\,^3D$. Thus, it is evident that 6° is a valid level, but there is no corresponding experimental level with J-value of 3 to which it can be assigned. An examination of the identified lines of Ni I, [10], reveals that the only transition of the level 6° with an even level of J-value 4 is the weak line $a\,^3F_4-6^\circ$ at 49032. However, *this* line was measured by Shenstone in the spectrum of Ni II, [15]. Then neglecting the above transition, the level 6° can be assigned to $^3P(^3P)^1D$, as indicated above.

Below 54000, (the limit of the experimental data available), there are 10 theoretical levels with no corresponding experimental levels. The lowest of these is the level $^3P(^3P)^5P_1$ at 40695.

As mentioned previously, whenever there is more than one experimental source for the g-factors, the

agreement is usually very good between the various values obtained. The only exceptions are the g-factors of the levels $y\,^3F_2$ and $y\,^3D_2$, which were measured by Lindsley, [14], and Marvin and Baragar, [12]. Lindsley's value of 0.973 for $y\,^3F_2$ is based on 6 separate lines with 14 measurements taken, and his value of 0.859 for $y\,^3D_2$ is also based on 6 separate lines with 19 measurements taken. In only one of these 12 lines is the g-factor for the even level assumed. The experimental values of 0.79 and 1.19 obtained for the g-factors of $y\,^3F_2$ and $y\,^3D_2$ by Marvin and Baragar are based on only two lines in each case. Although for these two levels the g-factors of Marvin and Baragar are quoted in AEL, it seems evident that Lindsley's values are more reliable and should be adopted. This assumption is verified by the calculated g-factors obtained in the present investigation. For the theoretical levels $^3F(^3P)^3F_2$ and $^3F(^3P)^3D_2$, the g-factors of 0.903 and 0.929, respectively, are obtained to which Lindsley's values fit much better than those of Marvin and Baragar.

With the exception of the g-factors for $y\,^3P_1$, $w\,^3F_3$ and $y\,^3G_3$, discussed previously, the agreement between the experimental and calculated g-factors is very good.

The calculated values, percentage compositions and g-factors of all the 114 predicted levels (50 terms) of $3d^94p + 3d^84s4p + 3d^95p$ are given in table A.

It is interesting to note that the rms error of 131 for the configurations $(3d+4s)^94p$ is lower than the present value of 147. The difference between the rms deviations is not so large, since for $(3d+4s)^94p$ there are 17 free parameters for 71 levels yielding an rms deviation of 114, whereas for $3d^94p + 3d^84s4p + 3d^95p$, there are 25 free parameters for 83 levels giving an rms deviation of only 122.

Finally, the rms error of 147 obtained here should be compared with the rms errors of 173 for $3d^94p + 3d^84s4p$ and 139 for $3d^95p$. Since the configuration $3d^95p$ lies within the range of the observed levels of $3d^84s4p$ a greater improvement may have been expected. However, from table A it is apparent that although the eigenfunctions of the levels of $3d^94p$ are mixed considerably, the mixing is mostly among eigenfunctions belonging to $3d^95p$. Only the eigenfunctions of two levels from $3d^84s4p$ comprise contributions of more than 15 percent belonging to $3d^95p$. These are the levels $^1G(^3P)^3F_{2,3}$. Although for $(3d+4s)^94p$ the mean deviation for the levels of $^1G(^3P)^3F$ is only 109, in the present case the mean deviation is reduced to 13.

Appendix

Table A. Observed and Calculated Levels and g-Factors

In the column "Name" the calculated designation of the term is given. The terms of d^8sp are denoted by $d^8v_1S_1L_1\ (sp^{1,3}P)SL$.

The entries in the columns "J", "Obs. Level (cm^{-1})", "Calc. Level (cm^{-1})", "Obs. g-Factor" and "Calc. g-Factor" are self-evident. In the column "Percentage" for each calculated level either the three highest contributions or all those contributions exceeding five percent are given.

Whenever the experimental and calculated term designations differ, the experimental designation is entered in the column "AEL", with the notation of C. E. Moore, [1]. In many instances the exchanges involve complete terms rather than isolated levels. Unless specified otherwise, the entries in the column "AEL" pertain to exchanges in terms.

The column "O−C" gives the difference between the observed and calculated values of the levels.

The entries are in increasing energy of the calculated values.

TABLE A. *Observed and calculated levels of* Ni I $3d^94p + 3d^84s4p + 3d^95p$

Name	J	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O−C	Obs. g-Factor	Calc. g-Factor
			Config.	Desig.					
$^3F(^3P)^5D$	0	96	$3d^84s(a\,^4F)4p$	$z\,^5D$	28213	28241	−28		
	1	95			27944	28008	−64	1.486	1.486
	2	94			27415	27551	−136	1.49	1.488
	3	94			26666	26906	−240	1.50	1.492
	4	96			25754	26119	−365	1.51	1.497
$^3F(^3P)^5G$	2	96	$3d^84s(a\,^4F)4p$	$z\,^5G$	29013	28856	157	0.364	0.359
	3	$90+6\,^3F(^3P)^5F$			28578	28473	105	0.945	0.938
	4	$87+8\,^3F(^3P)^5F$			28068	28015	53	1.171	1.165
	5	$88+10\,^3F(^3P)^5F$			27580	27543	37	1.28	1.277
	6	100			27261	27151	110	1.32	1.333
$^3F(^3P)^5F$	1	97	$3d^84s(a\,^4F)4p$	$z\,^5F$	30392	30231	161	0.006	0.020
	2	$72+9(^2D)4p\,^3D+7(^2D)4p\,^1D$			30163	30030	133	0.985	1.012
	3	$84+5\,^3F(^3P)^5G$			29833	29658	175	1.208	1.219
	4	$76+9(^2D)4p\,^3F+8\,^3F(^3P)^5G$			29084	29094	−10	1.288	1.317
	5	$90+8\,^3F(^3P)^5G$			28542	28490	52	1.38	1.386

TABLE A. *Observed and calculated levels of* Ni I $3d^94p + 3d^84s4p + 3d^95p$ – Continued

Name	J	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O–C	Obs. g-Factor	Calc. g-Factor
			Config.	Desig.					
$(^2D)4p\,^3P$	0	96			30192	30183	9		
	1	$87 + 5(^2D)4p\,^3D$			29501	29498	3	1.426	1.420
	2	$91 + 4(^2D)4p\,^3D$			28569	28590	−21	1.485	1.481
$(^2D)4p\,^3F$	2	$72 + 10\,^3F(^3P)^3F + 6(^2D)4p\,^3D$			30619	30655	−36	0.740	0.742
	3	$48 + 27(^2D)4p\,^1F + 8(^2D)4p\,^3D$			29321	29323	−2	1.086	1.087
	4	$79 + 12\,^3F(^3P)^5F + 6\,^3F(^3P)^3F$			29481	29419	62	1.287	1.263
$(^2D)4p\,^3D$	1	$59 + 30\,^3F(^3P)^3D$			30913	30919	−6	0.552	0.564
	2	$28 + 22\,^3F(^3P)^5F + 17(^2D)4p\,^1D$			29888	29893	−5	1.044	1.021
	3	$59 + 24\,^3F(^3P)^3D + 11(^2D)4p\,^1F$			29669	29760	−91	1.300	1.290
$(^2D)4p\,^1F$	3	$52 + 34(^2D)4p^3F$			31031	31021	10	1.048	1.049
$(^2D)4p\,^1D$	2	$61 + 17(^2D)4p\,^3D + 12\,^3F(^3P)^3D$			31442	31418	24	1.060	1.060
$^3F(^3P)^3G$	3	95	$3d^84s(a\,^2F)4p$	$z\,^3G$	31786	31765	21	0.761	0.763
	4	91			30980	31061	−81	1.052	1.049
	5	96			30923	30917	6	1.21	1.203
$(^2D)4p\,^1P$	1	95			32982	32983	−1	1.005	1.008
$^3F(^3P)^3F$	2	$49 + 35\,^3F(^3P)^3D$	$3d^84s(a\,^2F)4p$	$y\,^3D$	34163	34096	67	0.859	0.903
	3	$43 + 29\,^3F(^3P)^3D$	$3d^84s(a\,^2F)4p$	$y\,^3F$	33112	33197	−85	1.193	1.181
	4	86			32973	32994	−21	1.22	1.216
$^3F(^3P)^1G$	4	$72 + 13\,^3F(^3P)^3G + 12\,^3F(^3P)^3F$	$3d^84s(a\,^2F)4p$	$z\,^1G$	33590	33619	−29	1.035	1.043
$^3F(^3P)^3D$	1	$69 + 27(^2D)4p\,^3D$	$3d^84s(a\,^2F)4p$	$y\,^3D$	34409	34410	−1	0.511	0.507
	2	$31 + 39\,^3F(^3P)^3F + 17(^2D)4p\,^3D$	$3d^84s(a\,^2F)4p$	$y\,^3F$	33611	33622	−11	0.973	0.929
	3	$45 + 32\,^3F(^3P)^3F$	$3d^84s(a\,^2F)4p$	$y\,^3D$	33501	33511	−10	1.198	1.219
$^3F(^3P)^1F$	3	$84 + 10\,^3F(^3P)^3F$	$3d^84s(a\,^2F)4p$	$y\,^1F$	35639	35723	−84	1.013	1.014
$^3F(^3P)^1D$	2	$82 + 8(^2D)4p\,^1D$	$3d^84s(a\,^2F)4p$	$y\,^1D$	36601	36480	121	1.013	1.012
$^3P(^3P)^5P$	1	96				40695			2.456
	2	92		2°	40484	40458	26		1.796
	3	$90 + 8\,^1D(^3P)^3D$		1°	40361	40287	74		1.633
$^1D(^3P)^3D$	1	$75 + 10\,^3F(^3P)^3D$	$3d^84s(b\,^2D)4p$	$y\,^3P$	42656	42619	37	(1.32)	0.643
	2	$68 + 12\,^3F(^3P)^3D$			42654	42590	64		1.202
	3	$41 + 39\,^3F(^3P)^3D$	$3d^84s(b\,^2D)4p$	$x\,^3D$	42621	42418	203		1.354
$^1D(^3P)^3F$	2	$80 + 4\,^3P(^3P)^5D$	$3d^84s(b\,^2D)4p$	$x\,^3D$	42954	42976	−22	0.840	0.744
	3	$66 + 20\,^3P(^3P)^5D$	$3d^84s(a\,^4F)4p$	$w\,^3D$	42768	42822	−54	1.22	1.189
	4	$53 + 39\,^3P(^3P)^5D$	$3d^84s(b\,^2D)4p$	$x\,^3F$	42585	42595	−10	1.35	1.349
$^1D(^3P)^3P$	0	$62 + 32\,^3P(^3P)^3P$				43079			
	1	$59 + 23\,^3P(^3P)^3P + 8\,^1D(^3P)^3D$	$3d^84s(b\,^2D)4p$	$y\,^1P$	43464	43464	0	1.39	1.418
	2	$44 + 27\,^3P(^3P)^5D + 12\,^3P(^3P)^3P$	$3d^84s(b\,^2D)4p$	$x\,^1D$	43933	43915	18	1.48	1.457

TABLE A. *Observed and calculated levels of* Ni I $3d^94p + 3d^84s4p + 3d^95p$ — Continued

Name	J	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O−C	Obs. g-Factor	Calc. g-Factor
			Config.	Desig.					
$^3P(^3P)^5D$	0	91				44134			
	1	89				44094			1.485
	2	$56 + 27\,^1D(^3P)^3P$				44061			1.461
	3	$58 + 17\,^1D(^3P)^3D + 11\,^1D(^3P)^3F$	$3d^84s(b\,^2D)4p$	$x\,^1F$	44206	44159	47		1.401
	4	$34 + 30\,^3F(^1P)^3F + 21\,^3F(^1P)^3G$				44000			1.294
$^3F(^1P)^3G$	3	91	$3d^84s(a\,^4F)4p$	$w\,^3F$	44565	44411	154	(1.04)	0.784
	4	$72 + 24\,^3F(^1P)^3F$	$3d^84s(a\,^4F)4p$	$y\,^3G$	44315	44567	−252	1.18	1.289
	5	100			43090	42572	518	1.23	1.200
$^3F(^1P)^3D$	1	$67 + 11\,^3P(^3P)^3D$	$3d^84s(a\,^4F)4p$	$w\,^3D$	45122	45008	114	0.57	0.471
	2	$56 + 15\,^1D(^3P)^3D$			44475	44479	−4	1.16	1.172
	3	$34 + 29\,^1D(^3P)^3D + 16\,^3P(^3P)^5D$	$3d^84s(b\,^2D)4p$	$x\,^3F$	43655	43774	−119	1.24	1.317
$^3F(^1P)^3F$	2	86	$3d^84s(a\,^4F)4p$	$w\,^3F$	45419	45902	−483	0.68	0.668
	3	77	$3d^84s(a\,^4F)4p$	$y\,^3G$	45281	45300	−19	(0.78)	1.059
	4	$36 + 30\,^1D(^3P)^3F + 22\,^3P(^3P)^5D$	$3d^84s(a\,^4F)4p$	$w\,^3F$	43259	43501	−242	1.25	1.112
$^3P(^3P)^3P$	0	$63 + 30\,^1D(^3P)^3P$	$3d^84s(a\,^4P)4p$	$x\,^3P$	47687?	47660	27		
	1	$47 + 19\,^3P(^3P)^3D + 17\,^1D(^3P)^3P$			47208	47254	−46		1.203
	2	$59 + 18\,^3P(^3P)^5S$			46523	46609	−86		1.573
$^3P(^3P)^3D$	1	$66 + 14\,^3P(^3P)^3P$	$3d^84s(a\,^4P)4p$	$v\,^3D$	47425	47448	−23	0.726	0.727
	2	81			47139	47209	−70	1.209	1.170
	3	90			47030	47052	−22	1.331	1.323
$^3P(^3P)^5S$	2	$76 + 9\,^3P(^3P)^3P + 8\,^1D(^3P)^3P$		4°	47329	47517	−188		1.874
$(^2D)5p\,^1F$	3	$56 + 35(^2D)5p\,^3F$	$3d^9(a\,^2D)5p$	$v\,^3F$	48672	48677	−5		1.052
$^3P(^3P)^1P$	1	$83 + 6(^2D)5p\,^1P$		5°	48818	48727	91		1.063
$(^2D)5p\,^1D$	2	$47 + 17(^2D)5p\,^3P + 12\,^3P(^3P)^1D$	$3d^9(a\,^2D)5p$	$u\,^3D$	49185	49003	182		1.123
$^3P(^3P)^1D$	2	$75 + 11(^2D)5p\,^1D$		6°	49033	49137	−104		1.030
$(^2D)5p\,^3P$	0	$91 + 8\,^3P(^3P)^3P$			50139	50159	−20		
	1	$62 + 22(^2D)5p\,^1P + 7\,^3P(^3P)^3P$			49403	49238	165		1.374
	2	$65 + 19(^2D)5p\,^1D + 8\,^3P(^3P)^3P$			48735	48704	31		1.403
$^1G(^3P)^3H$	4	100				49553			0.800
	5	100				49653			1.034
	6	100				49778			1.167
$(^2D)5p\,^3F$	2	$57 + 30\,^1G(^3P)^3F$			50039	49937	102		0.662
	3	$23 + 24(^2D)5p\,^3D + 24(^2D)5p\,^1F$	$3d^9(a\,^2D)5p$	$w\,^1F$	50143	50074	69		1.138
	4	$84 + 13\,^1G(^3P)^3F$			48715	48792	−77		1.251
$^3P(^3P)^3S$	1	98				49928			1.986
$(^2D)5p\,^3D$	1	$80 + 10\,^3F(^1P)^3D$			50851	50929	−78		0.508
	2	$69 + 11(^2D)5p\,^1D + 11\,^3F(^1P)^3D$	$3d^9(a\,^2D)5p$	$w\,^1D$	50689	50674	15		1.130
	3	$59 + 14(^2D)5p\,^1F + 11(^2D)5p\,^3F$			49328	49423	−95		1.223
$(^2D)5p\,^1P$	1	$64 + 26(^2D)5p\,^3P$			50458	50519	−61		1.150

TABLE A. *Observed and calculated levels of* Co I $(3d+4s)^8 4p$ – Continued

Name	J	Percentage	AEL		Obs. Level (cm^{-1})	Calc. Level (cm^{-1})	O–C	Obs. g-Factor	Calc. g-Factor
			Config.	Desig.					
$^1G(^3P)^3F$	2	$57+32(^2D)5p\ ^3F+6^3F(^1P)^3F$	$3d^84s(a\ ^2G)4p$	$u\ ^3F$	51344	51337	7		0.662
	3	$61+27(^2D)5p\ ^3F+7^3F(^1P)^3F$			51125	51139	−14		1.081
	4	$81+12(^2D)5p\ ^3F$			50790	50808	−18		1.246
$^3P(^3P)^1S$	0	99				51726			
$^1G(^3P)^3G$	3	100				54106			0.750
	4	100				54129			1.050
	5	100				54152			1.200
$^1D(^1P)^1F$	3	$87+9^3P(^1P)^3D$				56358			1.034
$^3P(^1P)^3P$	0	93				57919			
	1	$69+21^1D(^1P)^1P$				57337			1.379
	2	$47+44^1D(^1P)^1D$				56671			1.259
$^1D(^1P)^1D$	2	$46+47^3P(^1P)^3P$				58144			1.257
$^1D(^1P)^1P$	1	$66+24^3P(^1P)^3P$				58832			1.140
$^3P(^1P)^3D$	1	95				59750			0.514
	2	95				59533			1.164
	3	$89+8^1D(^1P)^1F$				59274			1.303
$^3P(^1P)^3S$	1	98				62691			1.980
$^1G(^1P)^1H$	5	100				63188			1.000
$^1G(^1P)^1F$	3	93				64652			1.009
$^1G(^1P)^1G$	4	100				67640			1.000
$^1S(^3P)^3P$	0	99				80851			
	1	99				80934			1.500
	2	99				81103			1.500
$^1S(^1P)^1P$	1	99				94586			1.000

References

[1] Moore, C. E., Atomic energy levels, Nat. Bur. Stand. (U.S.), Circ. 467, Vol. II (1952). Referred to as AEL.
[2] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **73A** (Phys. and Chem.), No. 5, 497 (1969).
[3] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **74A** (Phys. and Chem.), No. 2, 141 (1970).
[4] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **74A** (Phys. and Chem.), No. 2, 157 (1970).
[5] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **74A** (Phys. and Chem.), No. 4, 507 (1970).
[6] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **74A** (Phys. and Chem.), No. 2, 181 (1970).
[7] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **74A** (Phys. and Chem.), No. 5, 703 (1970).
[8] Roth, C., J. Math. Phys. **9**, No. 5, 686 (1968).
[9] Roth, C., J. Res. Nat. Bur. Stand. (U.S.), **73A** (Phys. and Chem.), No. 6, 599 (1969).
[10] Russell, H. N., Phys. Rev. **34**, 821 (1929).
[11] Bakker, Proc. Akad. Amsterdam **35**, 82 (1932).
[12] Marvin, H. H., and Baragar, A. E., Phys. Rev. **43**, 973 (1933).
[13] Dijkstra, H., Physica **4**, 81 (1937).
[14] Lindsley, C. H., J. Opt. Soc. Am. **32**, 94 (1942).
[15] Shenstone, A. G., Phys. Rev. **30**, 255 (1927).

(Paper 74A5–636)