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COULOMB DISPLACEMENT ENERGIES IN THE $1f_{\frac{7}{2}}$ SHELL

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Abstract: The experimental Coulomb displacement energies in the $1f_{\frac{7}{2}}$ shell (except one) can be described by Hecht's Coulomb energy equation with a standard deviation of 8.5 keV if it is assumed that the Coulomb interaction radius is 2.6 ± 0.5 % larger for the completely filled shell than it is for the unfilled shell. The standard error of the calculated energies is 1.8 keV. Electromagnetic spin-orbit effects are indicated. The two Coulomb interaction energies V_0 and $\bar{V}_{\text{even}}$ which were obtained from the least-squares analysis are in very good agreement with the theoretically predicted values. The energy of the 0^+, $T = 1$ ground state of ^{42}Sc is too low and deviates by about 45 keV from the expected value.

1. Introduction

There exist various approaches for discussing the experimental Coulomb displacement energies. One approach makes use of so-called energy relationships [1]). Another widely used method consists in comparing the data with Coulomb energy equations. These equations range in character from empirical or semi-empirical to theoretical. The approach taken in the present study is close to the last case.

Coulomb displacement energies usually depend on N (isotope effect) and on the configurations of the corresponding states. These effects were studied recently [2-4]) for the Coulomb displacement energies in or including the $1f_{\frac{7}{2}}$ shell. Harchol *et al.* [2]) discussed the experimental data in terms of the Coulomb energy expression of Carlson and Talmi [5]). This equation was derived with harmonic oscillator wave functions but only for protons in a given shell ††. In the $1f_{\frac{7}{2}}$ shell, Harchol *et al.*[2]) used a harmonic oscillator constant which depends slightly on the number of neutrons in the shell. They found good agreement with the experimental results except for the three cases with $Z'_< =$ odd and $T > 1$ where they assumed a proton seniority of 2. Sherr [3]) also discussed the experimental data in terms of the Coulomb energy expression of Carlson and Talmi [5]), but in order to apply this equation to more general configurations he used a modified pairing term [7,8]) with a T-dependence of the form $1/T$. He found good agreement and essentially no explicit N-dependence (apart from the effect of the T-dependent pairing term). Nolen *et al.* [4]) studied the Coulomb displacement energies of the Sc-Ca isobaric pairs. They calculated wave functions in a Woods-Saxon

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†† Unna [6]) calculated Coulomb energy differences for the mirror nuclei and obtained results which were very close to the values from the expression of Carlson and Talmi [5]).

well. By simultaneously varying the depth and the radius of the well, they could fit the known binding energies of the excess neutrons and the observed Coulomb displacement energies. Except for $A = 42$, they found that the well radius follows a $A^{\frac{1}{3}}$ dependence very closely. The authors point out [see also ref. [9])] that this result implies that the proton mass distribution increases less rapidly than $A^{\frac{1}{3}}$.

The present investigation was motivated by the desire to learn more about the Coulomb displacement energies in the $1f_{\frac{7}{2}}$ shell by applying the new theoretical equations derived by Hecht [10-12]). These equations were obtained by taking into consideration isospin T in complete generality. It was hoped that the experimental data could be described to a considerably higher degree of accuracy and that information could be obtained about the A-dependence of the proton-proton Coulomb interaction radius. Both expectations were confirmed.

2. Hecht's Coulomb energy equations

Hecht [10-12]) derived two sets of theoretical Coulomb energy equations for any number of protons and neutrons in a given shell. [For extensions to mixed configurations, see refs. [10-12]).] One set of equations was obtained in the j-j coupling low seniority coupling scheme [10,11]); the other set was obtained in the Wigner supermultiplet scheme [12]). The T-dependence of the equations is identical in the two schemes; the A-dependence is very similar. It therefore appears likely that the A- and T-dependence of nuclei which have intermediate coupling schemes can also be represented by the above equations.

The first set of equations will be applied to the $1f_{\frac{7}{2}}$ shell. The equations contain several quantities which depend on the Coulomb interaction energies. One such quantity is the core interaction term

$$a_c = \frac{1}{2j+1} \sum_{J,\, j_c} (2J+1) \langle (jj_c)J | \frac{e^2}{3r_{ij}} | (jj_c)J \rangle, \tag{1}$$

where $j = \frac{7}{2}$ and j_c must be taken from all lower shells. The wave functions are antisymmetrized. All other quantities a, b, c etc. depend on the four Coulomb interaction energies

$$V_J = \langle (f_{\frac{7}{2}})^2 J | \frac{e^2}{3r_{ij}} | (f_{\frac{7}{2}})^2 J \rangle, \tag{2}$$

with $J = 0$, 2, 4 and 6. Only two combinations of these energies are needed in the discussion of the states which have a lowest seniority of $v = 0$ or $v = 1$. This will be done since all the 24 presently known Coulomb displacement energies in the $1f_{\frac{7}{2}}$ shell involve states having components with $v < 2$. The two energies are V_0 and $\overline{V}_{\text{even}} = \frac{1}{28}(V_0 + 5V_2 + 9V_4 + 13V_6)$.

Hecht's equations for the vector and tensor Coulomb energies for the $1f_{\frac{7}{2}}$ shell read as follows:

$$v = 0 \qquad E_C^{(1)} = 3(a+a_c)+3b(n-8),$$
$$E_C^{(2)} = b+c+c\,\frac{121-(n-8)^2}{(2T-1)(2T+3)}, \tag{3}$$

$$v = 1 \qquad E_C^{(1)} = 3(a+a_c)+\left(3b+\frac{3c}{2T(T+1)}\right)(n-8)-(-1)^{\frac{1}{2}n-T}3c\,\frac{5(2T+1)}{T(T+1)},$$
$$E_C^{(2)} = b+c+c\,\frac{100-(n-8)^2}{4T(T+1)}, \tag{4}$$

with

$$n = A-40,$$
$$a = \tfrac{7}{2}\overline{V}_{\text{even}},$$
$$b = \tfrac{1}{12}(7\overline{V}_{\text{even}}-V_0),$$
$$c = \tfrac{7}{216}(V_0-\overline{V}_{\text{even}}). \tag{5}$$

It should be noted that the coefficients $\tilde{a}$, $\tilde{b}$ and $\tilde{c}$ in the isobaric multiplet mass equation $M(T_z) = \tilde{a}+\tilde{b}T_z+\tilde{c}T_z^2$ are closely related to $E_C^{(0)}$, $E_C^{(1)}$ and $E_C^{(2)}$. For $\tilde{b}$ and $\tilde{c}$, the relations are $\tilde{b} = \Delta m - E_C^{(1)}$ and $\tilde{c} = 3E_C^{(2)}$ with $\Delta m = 0.783$ MeV.

The ordinary Coulomb displacement energies between states of isospin T and with $T_z = T-1$ and $T_z = T$ can be obtained from the relation $\Delta E_C(A, T, T-1|T) = E_C^{(1)}(A, T)-3(2T-1)E_C^{(2)}(A, T)$. Any other Coulomb displacement energy (like ^{42}Ti–^{42}Sc or ^{42}Ti–^{42}Ca) can be obtained from the more general relation $\Delta E_C(A, T, T_z-k|T_z) = kE_C^{(1)}(A, T)-3k(2T_z-k)E_C^{(2)}(A, T)$ where k is an integer and $|T_z| \leqq T$, $|T_z-k| \leqq T$.

Hecht [10]) pointed out that for very precise determinations of the various parameters and of the Coulomb interaction energies V_J, one must take into account other small effects. One such effect is the electromagnetic spin-orbit interaction between nucleons. This effect can increase the above small pairing quantity c of eq. (5) by as much as 40 %. The increase in the tensor part should exceed the increase in the vector part by the factor $(g_p-g_n)/g_p \approx 1.7$. Therefore, the quantity c in eqs. (3) and (4) was replaced by the two quantities $c^{(1)}$ and $c^{(2)}$, respectively. The differences $c^{(1)}-c$ and $c^{(2)}-c$ represent the contributions from the electromagnetic spin-orbit interaction and from other small effects like charge dependent nuclear forces.

Using eqs. (3) and (4), one obtains for the ordinary Coulomb displacement energies the expressions

$$v = 0 \qquad \Delta E_C = \alpha+\beta Z'_< -\gamma^{(2)}\left[2T-1+\frac{121-(n-8)^2}{2T+3}\right], \tag{6}$$

$$v = 1 \qquad \Delta E_C = \alpha+\beta Z'_< +\gamma^{(1)}\left[\frac{n-8}{2T(T+1)}-(-1)^{Z'_<}\frac{5(2T+1)}{T(T+1)}\right]$$
$$-\gamma^{(2)}\left[2T-1+\frac{(2T-1)}{4T(T+1)}(100-(n-8)^2)\right], \tag{7}$$

with

$$\begin{aligned} Z'_< &= \tfrac{1}{2}n - T, \\ \alpha &= 3(a + a_c) - 21b, \\ \beta &= 6b, \\ \gamma^{(1)} &= 3c^{(1)}, \\ \gamma^{(2)} &= 3c^{(2)}. \end{aligned} \tag{8}$$

Eq. (7) shows that the oscillatory pairing term in odd-mass nuclei is only one of several small terms which contribute to ΔE_C. The T-dependence of the oscillatory pairing term is only approximately of the form $1/T$. The other small terms depend explicitly on $n = A - 40$ and T.

The parameters a_c, a, b, $c^{(1)}$ and $c^{(2)}$ are not necessarily constant but can depend on A. Often, however, it is tacitly assumed that they are constant because it appears more appropriate in shell-model calculations. One would therefore hope that the A-dependence of the above parameters (and of V_0 and $\overline{V}_{\text{even}}$) is weak.

A comparison between the experimental Coulomb displacement energies of the Sc–Ca isobaric pairs and the expression

$$\Delta E_C = \alpha - 18\gamma^{(2)} + \delta_{v1} \frac{18}{n} (\gamma^{(2)} - \gamma^{(1)}), \tag{9}$$

which is derived from eqs. (6) and (7) with $Z'_< = 0$ and $T = \frac{1}{2}n$ clearly shows that an A-dependence has to be introduced. It also shows that the (very small) oscillating term which is due to the electromagnetic spin-orbit interaction is not sufficient to explain the experimental ^{42}Sc–^{42}Ca Coulomb displacement energy. An anomaly for this isobaric pair has already been noticed by Nolen *et al.*[4]). In the subsequent analysis the ^{42}Sc–^{42}Ca and ^{42}Ti–^{42}Sc energies were excluded; the ^{42}Ti–^{42}Ca energy was not excluded.

3. The least-squares analysis

Eqs. (6) and (7) together with the remaining 23 experimentally known Coulomb displacement energies were used in a least-squares analysis [13]). The quantities α, β, $\gamma^{(1)}$ and $\gamma^{(2)}$ were treated as parameters. They were assumed to decrease with A according to $\alpha = \alpha_0(\frac{1}{40}A)^{-\frac{1}{3}\lambda}$ etc. or $\alpha = \alpha_0\,[1 + \frac{1}{3}\lambda \cdot \frac{1}{40}(A-40)]^{-1}$ etc. with λ as an additional parameter. The Coulomb interaction radii R_J with

$$\frac{1}{R_J} = \langle (f_{\frac{7}{2}})^2 J | \frac{1}{r_{ij}} | (f_{\frac{7}{2}})^2 J \rangle \tag{10}$$

therefore increase according to $R_J = R_{J0}(\frac{1}{40}A)^{\frac{1}{3}\lambda}$ or $R_J = R_{J0}[1 + \frac{1}{3}\lambda \cdot \frac{1}{40}(A-40)]$, where the R_{J0} are constant. The latter function contains only the leading linear term of the Taylor expansion of the former function. The parameter λ was varied between $\lambda = 0$ (R_J independent of A) and $\lambda = 1$ ($A^{\frac{1}{3}}$ dependence of R_J). Also, the parameters

$\gamma^{(1)}$ and $\gamma^{(2)}$ were taken to be equal (no electromagnetic spin-orbit interaction) or not necessarily equal. Fig. 1 shows the result of the least-squares fitting process. The quantity

$$\chi^2 = \sum_{i=1}^{23} \{[\Delta E_C(i, \text{calc}) - \Delta E_C(i, \text{exp})]/\sigma(i, \text{exp})\}^2 \tag{11}$$

is plotted as a function of the parameter λ. The $\sigma(i, \text{exp})$ are the quoted uncertainties of the experimental Coulomb displacement energies $\Delta E_C(i, \text{exp})$. For each value of λ, a search on the parameters α_0, β_0, $\gamma_0^{(1)}$ and $\gamma_0^{(2)}$ was performed to find

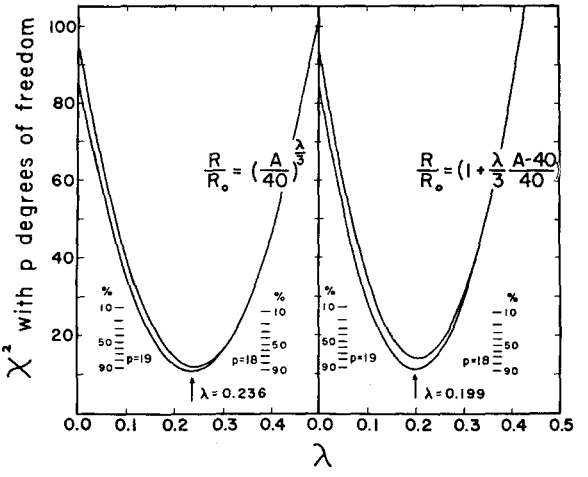

Fig. 1. Plot of the quantity $\chi^2 = \Sigma_{i=1}^{23}\{[\Delta E_c(i, \text{calc}) - \Delta E_c(i, \text{exp})]/\sigma(i, \text{exp})\}^2$ as a function of the parameter λ in the two expressions for the Coulomb interaction radius R. The respective lower (upper) curves were obtained with (without) the inclusion of electromagnetic spin-orbit effects. The number p of degrees of freedom is $p = 18$ ($p = 19$).

the values which minimize χ^2. Very pronounced minima clearly exist. The best agreement is obtained with the expression $R_J = R_{J0}(\frac{1}{40}A)^{\frac{1}{3}\lambda}$ and $\lambda = 0.236$. The corresponding values for α, β, $\gamma^{(1)}$ and $\gamma^{(2)}$ are shown in table 2. The uncertainties of these values will be explained later. The standard deviation

$$\sigma = \left\{ \frac{23}{23-5} \frac{\sum_{i=1}^{23} \{[\Delta E_C(i, \text{calc}) - \Delta E_C(i, \text{exp})]/\sigma(i, \text{exp})\}^2}{\sum_{i=1}^{23} \{1/\sigma(i, \text{exp})\}^2} \right\}^{\frac{1}{2}} \tag{12}$$

of the experimental energies $\Delta E_C(i, \text{exp})$ is $\sigma = 8.5$ keV; the standard error $\sigma_0 = \sigma/\sqrt{23}$ of the calculated energies $\Delta E_C(i, \text{calc})$ is $\sigma_0 = 1.8$ keV. The above value of λ corresponds to an increase in the Coulomb interaction radii R_J of 2.6 % within the $1f_{\frac{7}{2}}$ shell.

TABLE 1

Comparison between experimental and calculated Coulomb displacement energies in the $1f_{\frac{7}{2}}$ shell

Isobaric pair	A	T	$Z'_<$	ΔE_C(exp) [a] (keV)	ΔE_C(calc) (keV)	ΔE_C(calc) − ΔE_C(exp) (keV)
Sc–Ca	41	$\frac{1}{2}$	0	7282 ± 13	7287.1	5.1
	42	1	0	7214 ± 2 [b]	7258.8 [b]	44.8 [b]
	43	$\frac{3}{2}$	0	7244 ± 12	7250.2	6.2
	44	2	0	7229 ± 10	7232.2	3.3
	45	$\frac{5}{2}$	0	7231 ± 12	7222.4	−8.6
	46	3	0	7208 ± 10	7207.0	−1.0
	47	$\frac{7}{2}$	0	7194 ± 15	7196.9	2.9
	48	4	0	7175 ± 15	7182.9	7.9
Ti–Sc	43	$\frac{1}{2}$	1	7635 ± 20	7665.0	30.0
	44	1	1		[c]	
	45	$\frac{3}{2}$	1	7580 ± 30	7571.3	−8.7
	46	2	1		[c]	
	47	$\frac{5}{2}$	1	7560 ± 30	7536.6	−23.4
	48	3	1		[c]	
	49	$\frac{7}{2}$	1	7520 ± 30	7509.3	−10.7
V–Ti	45	$\frac{1}{2}$	2		7888.5	
	46	1	2	7835 ± 5	7829.4	−5.6
	47	$\frac{3}{2}$	2	7860 ± 30	7834.2	−25.8
	48	2	2	7815 ± 20	7818.3	3.3
	59	$\frac{5}{2}$	2	7796 ± 30	7814.1	18.1
	50	3	2	7805 ± 30	7801.5	−3.5
Cr–V	47	$\frac{1}{2}$	3		8263.8	
	48	1	3		[c]	
	49	$\frac{3}{2}$	3	8170 ± 100 [d]	8160.9	−9.1
	50	2	3		[c]	
	51	$\frac{5}{2}$	3	8130 ± 100 [d]	8132.9	2.9
Mn–Cr	49	$\frac{1}{2}$	4		8486.0	
	50	1	4	8412 ± 5	8419.7	7.7
	51	$\frac{3}{2}$	4		8431.6	
	52	2	4	8394 ± 40	8417.0	23.0
Fe–Mn	51	$\frac{1}{2}$	5		8859.0	
	52	1	5		[c]	
	53	$\frac{3}{2}$	5	8800 ± 70	8762.4	−37.6
Co–Fe	53	$\frac{1}{2}$	6		9079.9	
	54	1	6	9033 ± 5	9029.7	−3.3
Ni–Co	55	$\frac{1}{2}$	7		9450.8	
Ti–Sc	42	1		7769 ± 15 [b]	7716.8 [b]	−52.2 [b]
Ti–Ca	42	1		14983 ± 15 [e]	14975.6 [e]	−7.4 [e]

[a] Practically all experimental Coulomb displacement energies were taken from ref. [3]).

[b] Not included in the least-squares fit.

[c] See text and table 3.

[d] No experimental uncertainties were quoted in ref. [3]). Uncertainties of ±100 were arbitrarily assigned to these two values. The good agreement with the calculated values seems to indicate that the experimental uncertainties are much smaller.

[e] Included in the least-squares fit by using eq. (3).

4. Results and discussion

Table 1 shows a comparison between the individual experimental and calculated Coulomb displacement energies. The agreement is extremely good except for the two energies which depend on the energy of the 0^+, $T = 1$ ground state of ^{42}Sc. The experimental energy of this state is too low by about 45 keV; this is more than 20 times the experimental uncertainty and more than five times the standard deviation derived from all experimental energies. Nolen *et al.* [4]) pointed out that this deviation may possibly be caused by an isospin admixture because ^{42}Sc has $T_z = 0$ and the energy

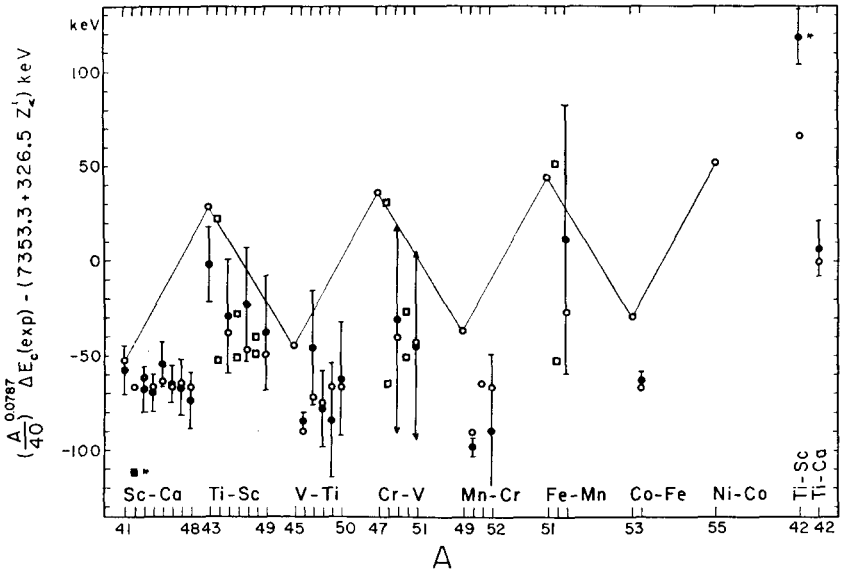

Fig. 2. Plot of the quantity $(\frac{1}{40}A)^{0.0787}\Delta E_C(\text{exp}) - (7353.3 + 326.5\, Z'_<)$ keV (filled circles) for the isobaric pairs in the $1f_{\frac{7}{2}}$ shell. For ^{42}Ti–^{42}Sc and ^{42}Ti–^{42}Ca corresponding quantities are plotted (see text). The open circles were calculated from eqs. (6) and (7) with the parameters $\gamma^{(1)}$ and $\gamma^{(2)}$ from table 2. The open squares were calculated with the Coulomb interaction energies V_J from table 2. The respective upper (lower) points represent the average for $J = 2, 4, 6$ ($J = 1, 3, 5, 7$). The two experimental energies marked with an asterisk deviate from the calculated values.

separation between $T = 0$ and $T = 1$ states of simple configurations is small. If this were the only reason for the above deviation, one would expect the same effect for the energy differences between ^{46}V–^{46}Ti, ^{50}Mn–^{50}Cr and ^{54}Co–^{54}Fe. This is not the case. The complete least-squares analysis was repeated with these additional (very accurate) Coulomb displacement energies excluded. The over-all fit is almost as good, and the three calculated energies are equally close to the experimental values. Therefore, it must be concluded that the effect applies specifically to this nucleus only. A low-lying state with 0^+, $T = 0$ and any configuration could certainly lead to isospin admixtures and thus depress the energy of the 0^+, $T = 1$ ground state of ^{42}Sc

which is the $T_z = 0$ member of the isobaric triplet. It is not quite clear, however, why such a 0^+, $T = 0$ state should not be present in any of the other odd self-conjugate nuclei. It should be pointed out that charge-dependent nuclear forces cannot be made responsible because they would not affect the general A- and T-dependence unless the interaction has a tensorial rank higher than 2. The above unexplained effect may have to be taken into account in the analyses of $0^+ \rightarrow 0^+$ superallowed β-transition [14]). It may also have to be considered in shell-model calculations (e.g. ref. [15]) and refs. quoted therein) for the $1f_{\frac{7}{2}}$ shell where the nucleus ^{42}Sc plays an important role.

Coulomb displacement energies ΔE_C are given by $\Delta E_C = \alpha + \beta Z'_< +$ small terms [see eqs. (6) and (7)]. To examine the fine structure effects due to the presence of the small terms one can compare the quantity $\Delta E_C(\text{exp}) - (\alpha + \beta Z'_<)$ with the small terms. This is done in fig. 2. For practical reasons, however, the factor $(\frac{1}{40}A)^{0.0787}$ is included. This factor, which amounts to at most 2.6 %, cancels the A-dependence of the parameters α, β, $\gamma^{(1)}$ and $\gamma^{(2)}$. Fig. 2 shows a plot of the quantity $(\frac{1}{40}A)^{0.0787}$ $\Delta E_C(\text{exp}) - (7353.3 + 326.5\, Z'_<)$ keV for the various isobaric pairs (filled circles). No apparent pattern seems to exist. However, when using the eqs. (6) and (7) with the parameters $\gamma^{(1)}$ and $\gamma^{(2)}$ of table 2, the open circles were obtained. They reproduce the experimental values extremely well. Disregarding ^{42}Sc only three of the 23 experimental Coulomb displacement energies deviate from the calculated values by more than the quoted experimental uncertainties. Fig. 2 includes calculated energies (open squares) for the six cases with A = even and $Z'_<$ = odd. Here, the Coulomb displacement energies depend on the spins of the respective states which may range from 1 to 7. Only two values are shown, however. The respective upper (lower) point represents the average for even (odd) J. The spread of the three (four) individual energies is only about ± 10 keV. The details of the calculations will be discussed later. Fig. 2 also includes a thin line which connects the calculated values for $T = \frac{1}{2}$. This line is unrelated to the preceding remarks. It demonstrates the known effect of the oscillating pairing term for the mirror nuclei.

The parameters α, β, $\gamma^{(1)}$ and $\gamma^{(2)}$ which were derived earlier can be used to calculate the quantities a, b, c etc. and the Coulomb interaction energies V_0 and $\overline{V}_{\text{even}}$. The quantities $a + a_c$, b, $c^{(1)}$ and $c^{(2)}$ follow directly from eqs. (8). The result is included in table 2. The quoted uncertainties will be explained below. At this point a difficulty arises because the experimental numbers do not permit the calculation of the pairing quantity c. One only knows that the relation $c < c^{(1)}$ must hold. Therefore, the theoretical ratios (see below) $c/c^{(1)}$ and $c/c^{(2)}$ were used to estimate c. This procedure seems to be justified because the theoretical and experimental ratios $c^{(2)}/c^{(1)}$ are in reasonable agreement and also because the result is not very sensitive to these ratios. A value for c was obtained (the uncertainty due to this procedure was estimated and included in table 2) and the remaining quantities a, a_c, V_0 and $\overline{V}_{\text{even}}$ were calculated from eqs. (5). The quantity a_c can be used to calculate the average Coulomb interaction $\overline{V}_c$ of one proton in the $1f_{\frac{7}{2}}$ shell with a single proton in the core. Assuming

that the matrix element in eq. (1) is independent of j_c and J it follows that $a_c = Z_0 \overline{V}_c$, where Z_0 is the number of protons in the core. The value for $\overline{V}_c$ is included in table 2.

TABLE 2
Coulomb energy parameters for the $1f_{\frac{7}{2}}$ shell

	Obtained from least-squares analysis		Calculated [a]) with harmonic oscillator potential
λ	0.236 ± 0.040		
$\Delta R/R$	2.6 ± 0.5 %		
α	7353.3 ± 6.0 keV		
β	326.5 ± 4.5 keV	$(40/A)^{0.0787}$	307.3 keV
$\gamma^{(1)}$	2.891 ± 0.068 keV		3.12 keV
$\gamma^{(2)}$	3.703 ± 0.135 keV		3.39 keV
$a+a_c$	2832.0 ± 7.2 keV		
a	397.6 ± 7.0 keV		375.0 keV
a_c	2434.4 ± 10.0 keV		
b	54.4 ± 0.7 keV		51.2 keV
c	0.929 ± 0.100 keV	$(40/A)^{0.0787}$	0.92 keV
$c^{(1)}$	0.964 ± 0.023 keV		1.04 keV
$c^{(2)}$	1.234 ± 0.045 keV		1.13 keV
$c^{(1)}-c$	0.035 ± 0.120 keV		0.12 keV
$c^{(2)}-c$	0.305 ± 0.140 keV		0.21 keV
$c^{(2)}/c^{(1)}$	1.28 ± 0.08		1.09
b/c	58.6 ± 7.2		55.7
V_0	142.3 ± 5.0 keV		135.5 keV
V_2	(122.9) keV		115.8 keV
V_4	(111.4) keV		105.0 keV
V_6	(109.4) keV	$(40/A)^{0.0787}$	103.1 keV
V_{even}	113.6 ± 2.0 keV		107.2 keV
V_c	121.7 ± 0.5 keV		

[a]) The calculations were performed by K. T. Hecht.

The uncertainties of the various quantities listed in table 2 are based on the following considerations. It appears that the standard procedures [13]) for the extraction of uncertainties cannot be applied for two reasons. One reason is that eqs. (6) and (7) contain the empirical function $R_J/R_{J0} = (\frac{1}{40}A)^{\frac{1}{3}\lambda}$. Fig. 1 shows a minimum of the quantity χ^2 for $\lambda = 0.236$. Using another empirical function with a linear radius increase according to $R_J/R_{J0} = 1 + (\frac{1}{3}\lambda)\frac{1}{40}(A-40)$ one obtains a minimum value of χ^2 which is only slightly larger. The minimum, however, occurs for a value of λ which is about 15 % smaller. The uncertainty of λ should therefore be given such that it reflects the uncertainty in the empirical function. The second reasons why the standard procedures cannot be applied is the fact that the χ^2 test seems to be too good. A value of 10.5 for χ^2 with 18 degrees of freedom corresponds to a probability of 91 % that, on repeating the measurements of all the 23 experimental energies, larger de-

viations from the calculated values would be observed. One may consider such a high probability as a fortunate coincidence. A more realistic explanation, however, can be given by assuming that all or some of the experimental uncertainties $\sigma(i, \mathrm{exp})$ have been overestimated. This assumption is confirmed by the rather large uncertainty $\Delta\lambda$ which one obtains [13]) from the χ^2 plot of fig. 1. Using the "golden rule" $\Delta\lambda = (\frac{1}{2}\partial^2\chi^2/\partial\lambda^2)^{-\frac{1}{2}}$ one obtains $\Delta\lambda = 0.087$. If we assume that χ^2 should not exceed the mean value of $p = 18$ [the internal and external errors become equal; see Birge [15])] or should not exceed the limiting value of $p+\sqrt{2}p = 24$, we obtain the values $\Delta\lambda = 0.076$ or $\Delta\lambda = 0.100$, respectively. If we assume that $P(\chi^2)$ should not be smaller than 50 % or 10 %, we obtain the values $\Delta\lambda = 0.072$ or $\Delta\lambda = 0.107$, respectively. All these estimates are too large. Systematic deviations between the calculated and experimental energies ΔE_C can definitely be recognized for the limiting values of λ. One way to solve this problem would be to decrease all experimental uncertainties $\sigma(i, \mathrm{exp})$ by a factor of 0.77 which would increase $\chi^2_{\min}$ to the expected mean value of $p = 18$. Even a factor of 0.66 would increase $\chi^2_{\min}$ only up to the limiting value of $p+\sqrt{2}p = 24$ which still represents an acceptable fit. The uncertainty $\Delta\lambda$ will then decrease accordingly. However, instead of introducing such correction factors it was decided to make a reasonable estimate on $\Delta\lambda$ directly by studying the systematic deviations between the calculated energies ΔE_C (which depend on λ) and the experimental energies ΔE_C. The result is $\lambda = 0.236 \pm 0.040$, where the uncertainty $\Delta\lambda = 0.040$ should have the character of a standard deviation. The uncertainties of the quantities α, β etc. were obtained directly from the computer output for the respective values of λ. The effect of the increased uncertainty of c which was mentioned before was taken into account.

Table 2 shows the Coulomb interaction energies V_0, $\overline{V}_{\mathrm{even}}$ and the related parameters which were obtained from the least-squares analysis. In addition, the values which were calculated using a harmonic oscillator potential are shown. The oscillator constant had a value $e^2\sqrt{(m\omega)}/(2\pi\hbar) = 300$ keV which was derived from $\hbar\omega = (41\ \mathrm{MeV})/A^{\frac{1}{3}}$ with $A = 48$. The Coulomb interaction energies V_0 and $\overline{V}_{\mathrm{even}}$ are in surprisingly good agreement with the values obtained from the least-squares analysis despite the fact that (i) the ground states in the $1f_{\frac{7}{2}}$ shell are not pure seniority states, and (ii) a harmonic oscillator potential was used rather than a Woods-Saxon well. Increasing the oscillator constant by 6 % at the beginning of the shell and by 3 % at the end of the shell would give agreement to within 1 keV. This result seems to indicate that Coulomb displacement energies are rather insensitive to the details of the wave function.

Calculated energies for the contributions $c^{(1)}-c$ and $c^{(2)}-c$ from the electromagnetic spin-orbit interaction are also included in table 2. The values obtained from the least-squares analysis are in reasonable agreement with the calculated values. The least-squares analysis cannot provide very accurate values because the effect is small and therefore the uncertainties are large. However, the presence of the effect can definitely be seen. On the other hand, the improvement of the fit between the experi-

mental energies and the calculated energies obtained by assuming $c^{(2)} > c^{(1)} > c$ or $c^{(2)} = c^{(1)} = c$ is insignificant. (The second case is not included in tables 1 and 2.) The ^{41}Sc–^{41}Ca isobaric pair is the only pair where the difference between the calculated energies amount to more than 10 keV. The calculated energies are 7287 keV (see table 1) and 7275 keV, respectively. The parameters a_c, a and b are practically identical in the two cases, the parameter c is about 30 % larger for the second case. The (apparent) Coulomb interaction energies become $V_0 = (152.0\ \text{keV})(\frac{1}{40}A)^{\frac{1}{3}\lambda}$, $\overline{V}_{\text{even}} = (115.1\ \text{keV})(\frac{1}{40}A)^{\frac{1}{3}\lambda}$ and $\overline{V}_c = (121.5\ \text{keV})(\frac{1}{40}A)^{\frac{1}{3}\lambda}$ with $\lambda = 0.242$.

It should be noted that other small effects like charge-dependent nuclear forces may also contribute to $c^{(1)}$ and $c^{(2)}$. A charge-symmetric charge-dependent nuclear force, for instance, would increase $c^{(2)}$ but would not affect $c^{(1)}$. The experimental values for $c^{(1)}$ and $c^{(2)}$ seem to support the existence of such forces.

TABLE 3

Calculated Coulomb displacement energies in the $1f_{\frac{7}{2}}$ shell with even A and $v > 0$

Isobaric pair	A	T	$Z'_<$	J^{π} a)	ΔE_C(calc) in keV						
					1^+	2^+	3^+	4^+	5^+	6^+	7^+
Ti–Sc	44	1	1	2^+	7563	7657	7573	7640	7579	7638	7568
Ti–Sc	46	2	1	4^+	7538	7577	7548	7565	7554	7564	7543
Ti–Sc	48	3	1	6^+	7515	7536	7525	7529	7530	7529	7520
Cr–V	48	1	3	$(4)^+$	8141	8258	8154	8240	8161	8237	8147
Cr–V	50	2	3	$6^{(+)}$	8130	8169	8141	8158	8146	8157	8136
Fe–Mn	52	1	5	6^+	8746	8866	8754	8848	8759	8846	8748

The energies depend on J.
a) Ref. [17]).

The fact that the experimental and calculated (including electromagnetic spin-orbit interaction) energies V_0 and $\overline{V}_{\text{even}}$ agree so well permits a reliable estimation of the individual energies V_2, V_4 and V_6. They are shown in table 2 in parentheses. These energies can be used to calculate the missing (see table 1) Coulomb displacement energies for the six cases with even A and $v > 0$. The computations are more involved [10]), and many small parameters have to be calculated. The Coulomb displacement energies for $J = 1$ to 7 are shown in table 3. Similar calculations may be carried out for all pairs of excited isobaric analogue states in the $1f_{\frac{7}{2}}$ shell which are based on $(1f_{\frac{7}{2}})^n$ configurations. The J-dependence is rather weak except for an even-J/odd-J effect which is particularly pronounced for $T = 1$. In fig. 2, the open squares are included which represent the calculated small terms averaged over all even J or all odd J. Formulae for a simplified treatment of all cases including the $v = 2$ case with even and odd J are given in appendix A.

Carlson and Talmi's equation [5]) follow from Hecht's general equations [10,11]) by specializing with $T = -T_z = \frac{1}{2}n$. Strictly speaking the former equation cannot be

applied to any pair of isobaric nuclei because at least one member contains neutrons outside the core. The relative success of the Carlson-Talmi expression, however, is well understood. Coulomb displacement energies depend strongly on the number of protons in a given shell. The presence of neutrons leads only to the small terms which have the pairing quantity c as a common factor. These terms replace the proton-proton pairing term in the expression given by Carlson and Talmi.

From the least-squares analysis, it is found that the Coulomb interaction radii R_J are not constant but increase slightly with A. The extreme cases where $R_J = \text{const}$ ($\lambda = 0$) or $R_J \propto A^{\frac{1}{3}}$ ($\lambda = 1$) are completely ruled out. For the filled shell, the R_J have increased by 2.6 ± 0.5 %. This increase is 24 % of the increase which would follow from $R_J \propto A^{\frac{1}{3}}$. The Coulomb interaction energies V_J and all the other parameters decrease by the same percentage. From the Coulomb interaction energies of table 2, one obtains

$$\left.\begin{aligned} R_0 &= 3.38 \text{ fm} \\ R_2 &= 3.91 \text{ fm} \\ R_4 &= 4.31 \text{ fm} \\ R_6 &= 4.39 \text{ fm} \\ \bar{R}_c &= 3.95 \text{ fm} \end{aligned}\right\} (\tfrac{1}{40}A)^{0.0797}.$$

These radii are approximately equal to the nuclear radius. Such an A-dependence of R_J and the Coulomb interaction energies V_J is not an intrinsic constituent of the Coulomb energy eqs. (3) and (4). It is hoped that eventually this effect can be understood [9]) on more general grounds, in particular with regard to the differences between the radii of the proton and neutron mass distributions.

In summary, the preceding discussion has shown that excellent agreement exists between the experimental Coulomb displacement energies in the $1f_{\frac{7}{2}}$ shell and the values calculated from Hecht's Coulomb energy equations [10,11]). Even the Coulomb interaction energies V_0 and $\bar{V}_{\text{even}}$, which were calculated for a harmonic oscillator potential, are in very good agreement with the values obtained from the least-squares analysis. Electromagnetic spin-orbit effects are indicated. It is found that the Coulomb interaction radii R_J are not constant but increase slightly with A. The energy of the 0^+, $T = 1$ ground state of ^{42}Sc is about 45 keV too low for unknown reasons.

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Appendix A

AN APPROXIMATE FORMULATION OF HECHT'S COULOMB ENERGY EQUATIONS

The approximation

$$V_J = V + \delta_{J0}\Delta V \tag{13}$$

will be introduced. Thus, all Coulomb interaction energies V_J between pairs of protons are taken as equal except when their spins are coupled to $J = 0$. The quantity ΔV has the character of a Coulomb pairing energy. Electromagnetic spin-orbit effects will be neglected in this treatment. The above approximation results in a considerable simplification of the Coulomb energy equations, particularly for the cases with $A =$ even and $v > 0$. The J-dependence within the even-J and odd-J cases is removed. A small error is thereby introduced. Table 3 shows that the error for the Coulomb displacement energies in the $1f_{\frac{7}{2}}$ amounts to not more than 10 keV. An additional simplification of the equations is obtained by using an average Coulomb interaction energy $\overline{V}_c$ between a proton in the j-shell and a proton in the core by

$$\overline{V}_c = \frac{\sum_{J, j_c} (2J+1) V_J^{jj_c}}{\sum_{J, j_c} (2J+1)} . \tag{14}$$

The quantity a_c becomes $a_c = Z_0 \overline{V}_c$ where Z_0 is the number of protons in the core. All the other quantities a, b, c, d, e etc. [see ref. [11])] become simple functions of j, V and ΔV. For the vector, tensor and displacement energies, one obtains the following expressions:

$$E_C^{(1)}(n, T) = Z_0 3\overline{V}_c + \tfrac{1}{2}(n-1)3\left(V - \frac{\Delta V}{2j+1}\right) + \frac{j+1}{2j+1} 3\Delta V + f_1(n, T, j)3\Delta V, \tag{15}$$

$$E_C^{(2)}(n, T) = \frac{1}{2}\left(V - \frac{\Delta V}{2(2j+1)}\right) + f_2(n, T, j)3\Delta V, \tag{16}$$

$$\Delta E_C(n, T, T-1|T) = Z_0 3\overline{V}_c + (\tfrac{1}{2}n - T)3\left(V - \frac{\Delta V}{2j+1}\right) + \frac{4(j+1)-(2T-1)}{4(2j+1)} 3\Delta V + f_3(n_1 T, j)3\Delta V, \tag{17}$$

$$f_1(n, T, j) = \frac{1}{2(2j+1)} \begin{cases} 0, & \text{(18a)} \\ \dfrac{(n-2j-1)}{4T(T+1)} - (-1)^{\frac{1}{2}n-T} \dfrac{(2j+3)(2T+1)}{4T(T+1)}, & \text{(18b)} \\ 0, & \text{(18c)} \\ 4\dfrac{(n-2j-1)}{4T(T+1)}, & \text{(18d)} \end{cases}$$

$$f_2(n, T, j) = \frac{1}{12(2j+1)} \begin{cases} \dfrac{(2j+4)^2-(n-2j-1)^2}{(2T-1)(2T+3)}, & \text{(19a)} \\ \dfrac{(2j+3)^2-(n-2j-1)^2}{4T(T+1)}, & \text{(19b)} \\ \dfrac{(2j+2)^2-(n-2j-1)^2}{(2T-1)(2T+3)}, & \text{(19c)} \\ \dfrac{(2j+2)^2-(n-2j-1)^2}{(2T-1)(2T+3)}\left(1-\dfrac{3}{T(T+1)}\right)-\dfrac{1}{T(T+1)}, & \text{(19d)} \end{cases}$$

$$f_3(n, T, j) = f_1(n, T, j) - 3(2T-1) f_2(n, T, j), \qquad (20)$$

where the four cases correspond to

$$\begin{aligned} &A = \text{even}, && v \geqq 0, && J = 0, \\ &A = \text{odd}, && v \geqq 1, && \\ &A = \text{even}, && v \geqq 2, && J = 1, 3, \ldots, 2j, \\ &A = \text{even}, && v \geqq 2, && J = 2, 4, \ldots, 2j-1. \end{aligned}$$

A special example for an application of the above equations is given below. The slope and the amplitude of the oscillatory term of the vector Coulomb energies of the mirror nuclei [taken from table IV of ref. [8])] can be used to calculate V and ΔV. For the $1d_{\frac{5}{2}}$ shell, the result is $V = 134$ keV and $\Delta V = 51$ keV. These values can now be used to calculate the tensor Coulomb energies for the isobaric triplets. The result is

$A = 18$	$E_C^{(2)}(\text{calc}) = 92.4$ keV	$E_C^{(2)}(\text{exp}) = 103.7 \pm 1.0$ keV,
20	54.1 keV	56.8 ± 10.2 keV,
22	99.2 keV	102.2 ± 6.0 keV,
24	54.1 keV	52.7 ± 7.5 keV,
26	92.4 keV	101.3 ± 2.1 keV.

The comparison with the experimental values [taken from table I of ref. [8])] shows good agreement. In particular, the oscillations of $E_C^{(2)}$ are well reproduced. A full treatment as was done for the $1f_{\frac{7}{2}}$ shell, however, can be expected to give considerably better agreement. One would expect that in the p-shell and the ds shell, the "super-multiplet equations" are better than the "seniority equations".

Appendix B

CALCULATION OF UNKNOWN MASSES AND ISOBARIC ANALOGUE STATES

Eqs. (3) and (4) together with the parameters of table 2 can be used to calculate the masses of unknown proton-rich nuclei as well as the excitation energies of isobaric analogue states including higher isobaric analogue states.

TABLE 4

Calculated mass excesses ΔM for proton-rich nuclei in the $1f_{\frac{7}{2}}$ shell (in units of $\Delta M(^{12}C) = 0$)

Nucleus	ΔM(keV)	Nucleus	ΔM(keV)	Nucleus	ΔM(keV)
^{43}V	−17886± 7	^{49}Mn	−37687±11	^{51}Co	−27390±15
^{44}V	−23832±20	^{46}Fe	+ 648±15	^{52}Co	−34321±20
^{45}V	−31896± 5	^{47}Fe	− 7051±11	^{53}Co	−42401±45
^{44}Cr	−13451± 9	^{48}Fe	−18113± 8	^{48}Ni	+16524±18
^{45}Cr	−19568± 7	^{59}Fe	−25661± 8	^{49}Ni	+ 7678±15
^{46}Cr	−29527± 5	^{50}Fe	−34476± 5	^{50}Ni	− 4113±13
^{47}Cr	−34529± 8	^{51}Fe	−40184±50	^{51}Ni	−11983±10
^{45}Mn	− 5111±11	^{47}Co	+ 9718±15	^{52}Ni	−22694± 9
^{46}Mn	−12572±41	^{48}Co	+ 1050±60	^{53}Ni	−29654± 9
^{47}Mn	−22638± 6	^{49}Co	− 9908±10	^{54}Ni	−39302± 6
^{48}Mn	−29285±20	^{50}Co	−17663±14	^{55}Ni	−45346±11

TABLE 5

Calculated excitation energies for isobaric analogue states in the $1f_{\frac{7}{2}}$ shell

Nucleus	T_z	T	E_x (keV)	Nucleus	T_z	T	E_x (keV)
^{44}Ti	0	1	4726± 8	^{51}Mn	$\frac{1}{2}$	$\frac{5}{2}$	11115± 50
^{48}Cr	0	1	5968±200 [a]	^{46}Ti	1	3	14183± 10
^{52}Fe	0	1	5600± 15	^{48}V	1	3	13804± 22
^{51}Mn	$\frac{1}{2}$	$\frac{3}{2}$	4371± 50	^{50}Cr	1	3	13203± 6
^{46}Ti	1	2	9059± 7	^{47}Ti	$\frac{3}{2}$	$\frac{7}{2}$	15750± 8
^{50}Cr	1	2	8319± 7	^{49}V	$\frac{3}{2}$	$\frac{7}{2}$	15195± 8
^{48}Ti	2	3	10635± 9	^{48}Ti	2	4	17409± 10
^{44}Ti	0	2	9467± 13	^{46}V	0	3	15002± 14
^{46}V	0	2	9216± 23	^{48}Cr	0	3	20333±200 [a]
^{48}Cr	0	2	9030±200 [a]	^{50}Mn	0	3	13836± 30
^{50}Mn	0	2	8533± 34	^{47}V	$\frac{1}{2}$	$\frac{7}{2}$	20612± 12
^{52}Fe	0	2	8549± 14	^{49}Cr	$\frac{1}{2}$	$\frac{7}{2}$	20721± 14
^{45}Ti	$\frac{1}{2}$	$\frac{5}{2}$	11430± 7	^{48}V	1	4	21329± 12
^{47}V	$\frac{1}{2}$	$\frac{5}{2}$	11543± 10	^{48}Cr	0	4	27862±200 [a]
^{49}Cr	$\frac{1}{2}$	$\frac{5}{2}$	11245± 12				

[a] The estimated uncertainty is mostly due to the experimental uncertainty of the mass of ^{48}Cr. The estimated uncertainties of the differences between any two excitation energies are considerably smaller.

Table 4 shows the result for the masses of proton-rich nuclei. The values were calculated from the known masses [18]) of the higher-order mirror nuclei and the relation $\Delta E_C(n, T, -T_z|+T_z) = 2T_z E_C^{(1)}(n, T)$. For the odd-mass nuclei and the even nuclei, $E_C^{(1)}$ was calculated from eqs. (3) and (4). For the odd nuclei ^{44}V, ^{46}Mn, ^{48}Mn, ^{48}Co, ^{50}Co and ^{52}Co, the "J-independent" approximation was used [see ref. [12]) and appendix A] and J was assumed to be even. An additional uncertainty was introduced for these six cases. The quoted uncertainties of the calculated masses must be considered with caution, particularly for the nuclei far off the stability line.

There may be additional effects like the one observed in ^{42}Sc or the Thomas-Ehrman shift which are not included in the calculation. The nuclei which are unstable with respect to proton emission (^{47}Co, ^{48}Co, ^{49}Co, ^{50}Co and ^{45}Mn) or two-proton emission (^{48}Ni and ^{49}Ni) are likely to have masses which are slightly lower. The decay $^{49}\text{Ni} \rightarrow {}^{47}\text{Fe}+2\text{p}$ has a calculated Q-value of only $Q = 150 \pm 20$ keV which makes this nucleus a possible candidate for double proton decay [19]).

Table 5 shows the calculated excitation energies of isobaric analogue states with $T = |T_z| + k$, where $k = 1, 2, 3$ and 4. For the ordinary isobaric analogue states with $k = 1$, only those states are listed which are experimentally unknown. The procedure used to calculate the excitation energies is very similar to the one mentioned above. The mass values were taken from ref. [18]). The Coulomb displacement energies were calculated from $\Delta E_C(n, T, T_z - k|T_z) = kE_C^{(1)}(n, T) - 3k(2T_z - k)E_C^{(2)}(n, T)$. For $k = 1$, the values of ΔE_C were taken directly from tables 1 and 3. The previous remarks about the quoted uncertainties also apply to the values given in table 5. Isobaric analogue states which undergo a T-allowed particle decay are likely to have a somewhat lower excitation energy. Some of the listed states may also be fragmented.

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