Systematics of proton and diproton separation energies for light nuclei

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A simple method to estimate proton and two-proton separation energies of proton-rich nuclei is presented that is sufficiently accurate to allow the prediction of suitable candidates for observable diproton decay. The method is based on the systematics of measured particle separation energies. Predictions for proton-rich nuclei with $Z=18-24$ are compared with the results of previous calculations. [S0556-2813(97)05610-0]

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I. INTRODUCTION

Diproton emission was first suggested as a possible exotic decay mode for proton-rich nuclei more than three decades ago by Goldansky [1]: A nucleus with an even number of protons may be more tightly bound than the nucleus with one fewer proton because of the pairing interaction, but unstable relative to the nucleus with two fewer protons because of the Coulomb interaction and symmetry energy. Recent experimental developments, especially the construction of radioactive beam facilities, permit the study of nuclei near or even beyond the limits of particle stability. But as yet, despite several experimental investigations (see, for example, Refs. [2,3]), no nuclides with $A>16$ have been observed to decay by direct diproton emission, although several nuclides, such as ^{22}Al and ^{31}Ar, are known to decay via the mechanism of β-delayed proton or diproton emission [4–6].

The requirements for the observation of direct diproton decay place rather severe restrictions on the lifetime of the diproton emitter. On the one hand, the parent nucleus must exist sufficiently long for it to be identified experimentally, although this obviously depends on the type of experiment. On the other hand, the lifetime for diproton emission must not be significantly longer than the lifetime of competing decay modes such as β^+ decay. According to Ormand [7], these constraints require that the lifetime for diproton emission be in the approximate range $10^{-8}-10^{-3}$ s. This in turn places very severe conditions on the allowed magnitude of the two-proton separation energy, because of the sensitivity of the Coulomb-barrier penetration probability, and hence the lifetime, to this quantity. Ormand [7] has estimated that in order that diproton decay be observable, the two-proton decay energy is limited to the range 0.9 to 1.4 MeV, although this range must, to some extent, be dependent on the charge of the nucleus.

One consequence of this limitation is that, in order to predict which nuclides are good candidates for observable diproton decay, it is necessary to employ calculational techniques that allow the two-proton separation energies to be determined with sufficient accuracy. In the past few years there have been a number of studies of proton-rich nuclei using various self-consistent mean-field theories [8–12], such as Skyrme-Hartree-Fock, Hartree-Fock-Bogoliubov, and the relativistic mean-field approximation. A second approach to computing ground-state binding energies is to utilize a mass formula; one sophisticated variant is the microscopic-macroscopic model developed by Möller and co-workers [13,14]. Although both these approaches give a reasonable global description of nuclear binding energies (and other nuclear properties), their usefulness in predicting two-proton separation energies is limited.

More successful in this respect are calculations [7,15–17] based on the nuclear shell model and the assumption of isobaric invariance of the strong interaction. In this approach the energy of a proton-rich nucleus (A,Z) is computed by adding to the measured energy of the analog neutron-rich nucleus $(A,A-Z)$ a calculated Coulomb energy difference $\Delta E_C(A,T)$; in terms of ground-state binding energies

$$B(A,T,T_3=-T)=B(A,T,T_3=T)-\Delta E_C(A,T), \quad (1)$$

where $T_3=(N-Z)/2$ is the third component of the isospin T. The accuracy achieved for calculated binding and separation energies is such that possible diproton emitters can be identified with reasonable certainty. In Ref. [17] the Coulomb energy difference is evaluated using a method based on a parameterization of the Coulomb displacement energies [19,20]. Alternatively, the Coulomb energy difference may be equated with $2b(A,T)T$ where the parameter $b(A,T)$ is defined by the isobaric mass multiplet equation,

$$B(A,T,T_3)=a(A,T)+b(A,T)T_3+c(A,T)T_3^2. \quad (2)$$

Brown [15] and Ormand [16,7] computed the $b(A,T)$ in shell-model calculations for fp-shell nuclei and nuclei at the interface between the sd and fp shells, using a Hamiltonian comprising isoscalar and isospin nonconserving parts [21,22].

In this paper a simplified version of the method of Ref. [17] is presented, in which one- and two-proton separation energies are deduced directly from measured ground-state binding energies. The accuracy achieved is comparable to that of Refs. [15–17,7], but the calculations are much easier to carry out. The method is illustrated for nuclei with charge $Z=18-24$ where a direct comparison is possible with the results of earlier work [15–17].

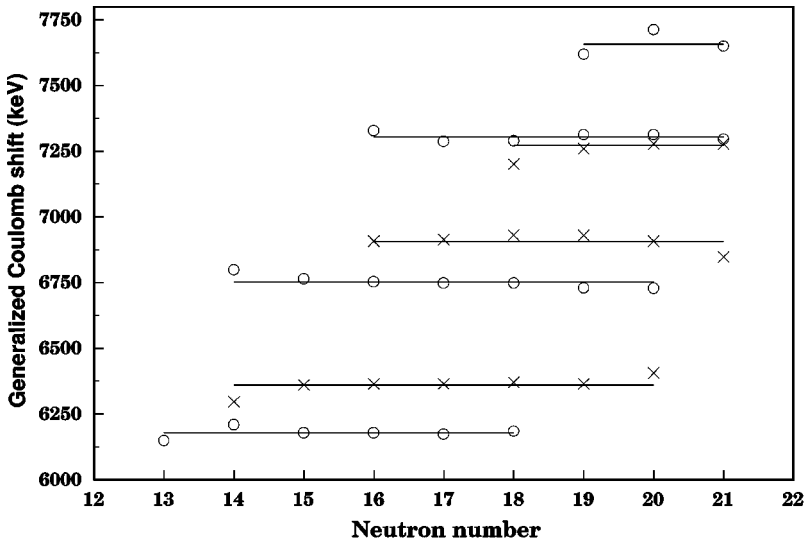

FIG. 1. Generalized Coulomb shift $\Delta_{np}(A,Z)$ for $Z=16-22$. The shifts, in keV, are smallest for $Z=16$ and largest for $Z=22$. The shifts deduced from experimental data are indicated by open circles (Z even) and crosses (Z odd), with average values shown as horizontal lines.

II. PROTON AND DIPROTON SEPARATION ENERGIES

We define a generalized Coulomb shift[1] $\Delta_{np}(A,Z)$ as the difference between the proton separation energy of a proton-rich[2] nucleus (A,Z) and the neutron separation energy of the analog neutron-rich nucleus $(A,A-Z)$:

$$\Delta_{np}(A,Z)\equiv S_n(A,A-Z)-S_p(A,Z), \tag{3}$$

where the separation energies are defined in terms of ground-state binding energies by

$$S_p(A,Z)=B(A,Z)-B(A-1,Z-1) \tag{4}$$

and

$$S_n(A,A-Z)=B(A,A-Z)-B(A-1,A-Z),$$

with an obvious change in notation from Eqs. (1) and (2). In an analogous manner we define a second generalized Coulomb shift,

$$\Delta_{2n2p}(A,Z)\equiv S_{2n}(A,A-Z)-S_{2p}(A,Z), \tag{5}$$

as the difference in the corresponding two-particle separation energies:

$$S_{2p}(A,Z)=B(A,Z)-B(A-2,Z-2) \tag{6}$$

and

$$S_{2n}(A,A-Z)=B(A,A-Z)-B(A-2,A-Z).$$

With these definitions the identity

$$\Delta_{2n2p}(A,Z)=\Delta_{np}(A,Z)+\Delta_{np}(A-1,Z-1) \tag{7}$$

is easily proved.

Explicit formulas for $\Delta_{np}(A,Z)$ and $\Delta_{2n2p}(A,Z)$ can be derived using a model for Coulomb energies developed in Refs. [19,20]. Consider a nucleus with N_π active protons and N_ν active neutrons in the valence orbital. The Coulomb energy of the nucleus, relative to the appropriate inert core, can be expressed [19] as

$$E_C(N_\pi,N_\nu)=N_\pi\varepsilon_C+\frac{1}{2}\,N_\pi(N_\pi-1)V_C+\left[\frac{1}{2}\,N_\pi\right]b_C+N_\pi N_\nu\gamma_C, \tag{8}$$

where $[\frac{1}{2}N_\pi]$ indicates the largest integer not exceeding $\frac{1}{2}N_\pi$ and, in the language of the shell model, ε_C, V_C, and b_C are the Coulomb parts of the single-particle energy, the average two-body matrix element, and the pairing energy, respectively. Specific expressions for V_C and b_C can be obtained within the seniority model [23], but here they may be regarded simply as parameters whose magnitudes are to be deduced by fitting measured Coulomb displacement energies. The additional term involving γ_C may be interpreted in several ways [19], but such a term essentially parametrizes in the simplest possible way the observed N_ν dependence of Coulomb displacement energies for fixed N_π. The extension of the model to situations in which active nucleons occupy two orbitals is discussed in Ref. [20], where the relevant equations may be found.

Within this model of Coulomb energies, the proton separation energy of a proton-rich nucleus (A,Z) may be expressed in terms of the neutron separation energy of the analog neutron-rich nucleus $(A,A-Z)$ and a difference in Coulomb energies. From Eqs. (1), (3), (4), and (8) we derive

$$\Delta_{np}(A,Z)=\varepsilon_C+(N_\pi-1)V_C+\frac{1}{2}(1+(-1)^{N_\pi})b_C. \tag{9}$$

[1]We use here the terminology introduced by Brown and Hansen [18] for the quantity which is more exactly the derivative of the Coulomb energy functional.

[2]In fact, all the equations in this section remain valid if the nucleus (A,Z) is neutron rich; we retain this terminology for convenience.

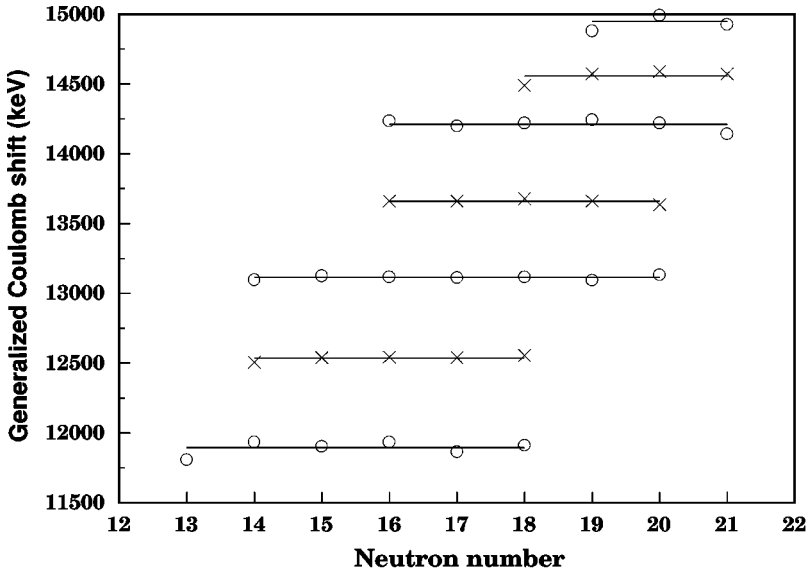

FIG. 2. Generalized Coulomb shift $\Delta_{2n2p}(A,Z)$ for $Z=16-22$. See the caption to Fig. 1.

Similarly, the two-proton separation energy of a nucleus may be expressed in terms of the two-neutron separation energy of the analog nucleus and a second difference in Coulomb energies, yielding

$$\Delta_{2n2p}(A,Z)=2\varepsilon_C+(2N_\pi-3)V_C+b_C. \qquad (10)$$

In Ref. [17] the Coulomb parameters ε_C, V_C, and b_C were determined in fits to measured Coulomb displacement energies, and Eqs. (9), (10) and the corresponding expression for $\Delta E_C(A,T)$ in Eq. (1) were used to predict binding energies and one- and two-proton separation energies for proton-rich nuclei with $Z=19-28$.

Although in deriving Eqs. (9) and (10) we have made use of the single-orbital version of the model, Eq. (8), they in fact remain valid even if the valence protons in the nucleus (A,Z) and its analog occupy different orbitals.[3] These equations contain no explicit or implicit dependence on N_ν; therefore, we may conclude that, within this model, the generalized Coulomb shifts $\Delta_{np}(A,Z)$ and $\Delta_{2n2p}(A,Z)$ for fixed Z are independent of mass. Goldansky [1] also suggested that $\Delta_{np}(A,Z)$ should be constant to within a few percent; he based his argument on an approximation to the liquid drop model. Note, however, that the interpretation of $\Delta_{np}(A,Z)$ as a generalized Coulomb shift is based upon the validity of Eq. (1); implicit in this equation is the assumption that the nuclear wave functions of analog states are identical. In particular, no account is taken of possible spreading of the charge distribution as, for fixed Z, the neutron number is decreased and the proton dripline is approached and passed. This results in a reduction in the Coulomb energy, the so-called Thomas-Ehrman shift [24–26]. Although one might expect rather large effects at the neutron dripline due to the spreading of the neutron distribution, at the proton dripline the effect should be diminished by the presence of the large Coulomb barrier, in addition to any centrifugal barrier.

The mass independence predicted by Eqs. (9) and (10) is also evident in the experimental data [27], as illustrated in Figs. 1 and 2 for nuclei with $Z=16-22$. Recently, Brown and Hansen [18] have noted that, for nuclei with $Z=13-16$, $\Delta_{np}(A,Z)$ is a smooth function of $S_p(A,Z)$ (and hence also of N_ν). Indeed, their plots show that $\Delta_{np}(A,Z)$ is approximately constant except, in the case of $Z=15$ and 16, for a decrease as S_p becomes negative.[4] As explained above, this behavior at the dripline is not unexpected, and indeed the effect should be most pronounced when the unbound proton has orbital angular momentum $l=0$, which is the situation for $Z=15$ and 16. There is little evidence for this effect in Figs. 1 and 2 because, with the exception of ^{39}Sc, none of the nuclei involved is beyond the dripline.

To investigate further the behavior of the generalized Coulomb shifts $\Delta_{np}(A,Z)$ and $\Delta_{2n2p}(A,Z)$ near the proton dripline we have performed a series of Skyrme-Hartree-Fock calculations [28,29]; in such calculations the mean field and, in particular, the charge distribution, can adjust dynamically to changes in (A,Z) as the dripline is approached. For open-shell nuclei we have adopted the ''filling'' approximation in an attempt to minimize problems associated with the BCS approximation when continuum states are involved. The detailed results obtained in Hartree-Fock calculations depend, of course, on the version of the Skyrme interaction used, although the trends should not; we have employed the interaction SkM1 [30]. We have computed $\Delta_{np}(A,Z)$ and $\Delta_{2n2p}(A,Z)$ for isotopes of argon with $A=29-47$, which

[3]Actually, if the nucleus (A,Z) has a single proton in the valence orbit Eq. (10) requires a slight modification. However, provided the orbital dependence of the parameters V_C and b_C is weak, this has negligible effect.

[4]For the most proton-rich nuclei, for which no measurements have been made, Brown and Hansen used masses deduced from systematics by Audi and Wapstra [27]. This could introduce rather large uncertainties in the Coulomb shift and perhaps introduce spurious behavior.

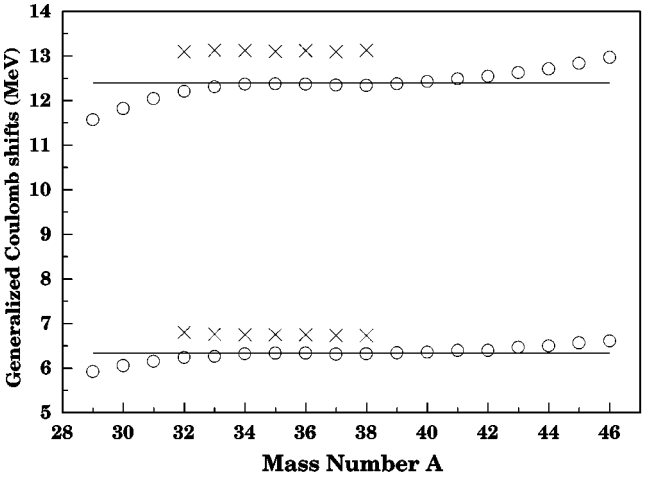

FIG. 3. Generalized Coulomb shifts $\Delta_{np}(A,Z)$ (lower values) and $\Delta_{2n2p}(A,Z)$ (upper values) for $Z=18$. The open circles represent the results of Skyrme-Hartree-Fock calculations, the lines are the calculated values averaged over mass number, and the crosses indicate experimental values. The shifts are in MeV.

requires the calculation of binding energies for almost 100 nuclides. With this interaction the nuclide ^{32}Ar is predicted to be just unbound to proton emission but just stable against diproton decay. The results of the calculations are summarized in Fig. 3; the open circles denote the calculated Coulomb shift, the horizontal lines show the calculated shifts averaged over A, and the crosses represent the experimental data [27]. In the rather limited mass range in which data are available, the mean-field calculations follow the observed trend, although both shifts are displaced by a few hundred keV from the data. A slight decrease in the magnitude of $\Delta_{np}(A,Z)$ beyond the proton dripline, due to the Thomas-Ehrman shift discussed above, is also evident; this decrease is magnified in the quantity $\Delta_{2n2p}(A,Z)$ as expected—see Eq. (7). The slight rise in $\Delta_{np}(A,Z)$ for large A is related to the decrease at small A, and is caused by the proton instability of the analog nuclides. The conclusion drawn from the Hartree-Fock calculations is that, for fixed Z, both generalized Coulomb shifts are approximately constant down to, and perhaps just beyond, the proton dripline. However, assuming $\Delta_{np}(A,Z)$ to be constant for smaller A leads to an underestimation of $S_p(A,Z)$ by an amount that grows as A decreases further.

The constancy of $\Delta_{np}(A,Z)$ for fixed Z suggests that $S_p(A,Z)$ and $S_{2p}(A,Z)$ can be predicted with reasonable accuracy for a given proton-rich nucleus (A,Z), provided that $\Delta_{np}(A',Z)$ is known experimentally for at least one nucleus (A',Z). We have adopted the following procedure for $Z=18-24$. First we have determined recommended values of $\Delta_{np}(A,Z)$ for each Z by selectively averaging the experimental data with respect to A'; corresponding values of $\Delta_{2n2p}(A,Z)$ are determined using Eq. (7). These recommended values are shown in Figs. 1 and 2 as horizontal lines. Then, using measured neutron and two-neutron separation energies for the analog nuclides, we have calculated proton and two-proton separation energies for several proton-rich nuclides for which no data are available. The results are

TABLE I. One-proton separation energies $S_p(A,Z)$ calculated for $Z=18-24$. The present calculations are compared with results from the references indicated. All energies are in keV with the estimated uncertainties given in parentheses.

Nucleus	Present	Cole [17]	Ormand [16]	Brown [15]	Systematics [27]
^{30}Ar	−465				350(355)
^{31}Ar	400				435(285)
^{32}K	−2725(90)				−1830(540)
^{33}K	−2425	−2447(31)			−1655(200)
^{34}K	−615	−639(26)			−610(300)
^{33}Ca	−1790(110)				
^{34}Ca	230	243(42)			900(355)
^{35}Ca	1085	1079(36)			1370(305)
^{37}Sc	−2965	−3006(26)	−2870(112)		−1990(300)
^{38}Sc	−1160	−1202(26)	−1144(86)	−1096(31)	−935(300)
^{38}Ti	375	368(30)	438(164)		1030(390)
^{39}Ti	415	405(29)	478(134)	439(36)	1120(315)
^{40}Ti	2210	2201(29)	2244(105)	2204(12)	1970(160)
^{42}V	−375	−376(26)	−312(105)	−303(40)	−255(200)
^{43}V	25	26(19)	89(63)	33(47)	190(235)
^{44}V	1790	1793(19)	1777(43)	1761(27)	1815(85)
^{41}Cr	−415(72)	−418(73)	−257(196)	−264(42)	
^{42}Cr	1155	1163(50)	1282(203)	1216(77)	1055(390)
^{43}Cr	1375	1375(31)	1448(134)	1398(65)	1255(215)
^{44}Cr	2860	2867(24)	2822(105)	2866(65)	2800(265)
^{45}Cr	3055	3060(50)	3078(76)	3083(47)	2855(130)

TABLE II. Diproton separation energies $S_{2p}(A,Z)$ calculated for $Z=18-24$. The present calculations are compared with results from the references indicated. All energies are in keV with the estimated uncertainties given in parentheses.

Nucleus	Present	Cole [17]	Ormand [16]	Brown [15]	Systematics [27]
^{30}Ar	−3105(67)				−1430(340)
^{31}Ar	−230				125(210)
^{32}K	−2330(90)				−1400(540)
^{33}K	25	17(52)			750(200)
^{34}K	2735	2726(50)			2730(300)
^{33}Ca	−4515(70)				
^{34}Ca	−2190	−2204(54)			−755(300)
^{35}Ca	455	440(52)			760(75)
^{37}Sc	−385	−371(44)	−309(107)		570(300)
^{38}Sc	1845	1854(44)	2358(84)	1927(23)	2090(300)
^{38}Ti	−2590	−2639(40)	−2432(132)		−960(255)
^{39}Ti	−750	−798(39)	−666(107)	−657(36)	185(105)
^{40}Ti	1540	1488(39)	1605(84)	1575(11)	1370(160)
^{42}V	2060	2051(40)	2142(84)	2105(39)	2220(195)
^{43}V	3845	3843(38)	3857(63)	3837(41)	3960(235)
^{44}V	6270	6268(38)	6265(26)	6248(26)	6305(85)
^{41}Cr	−2500(65)	−2498(52)	−2288(180)	−2249(79)	
^{42}Cr	−655	−647(58)	−452(151)	−498(67)	−260(340)
^{43}Cr	995	1000(43)	1136(122)	1095(52)	1000(95)
^{44}Cr	2885	2893(41)	2911(84)	2899(58)	2990(130)
^{45}Cr	4845	4853(41)	4855(63)	4844(40)	4670(105)

compared in Tables I and II with the predictions of previous calculations [15–17]. The uncertainties indicated for the results of the present calculations are due solely to the uncertainty in the measured neutron or two-neutron separation energies, and they are shown only if this exceeds 50 keV. The uncertainty in the recommended Coulomb shifts due to the averaging process is typically a few tens of keV or less, although this will certainly be increased by the extrapolation to the dripline; beyond the dripline systematic errors are introduced, as explained above. The agreement with the results of previous calculations is extremely good, although since all the calculational methods depend on the validity of Eq. (1), they all suffer the same defect beyond the proton dripline. To put the agreement between these calculations into perspective, we also include in the tables separation energies computed from the extrapolated masses of Ref. [27]; even allowing for the large uncertainties in the latter, large differences exist between these values and the results based on Eq. (1). Experimental information for nuclei near the proton dripline is scarce. The half-life of ^{30}Ar is known to be less than 20 ns, which is consistent with the predicted proton instability, whereas the observed β decay of ^{31}Ar confirms the predicted proton stability [2–6]; for a discussion of the decay modes of some isotopes of Ti and Cr, see Refs. [15–17].

III. DISCUSSION

We have suggested that proton and diproton separation energies for a proton-rich nucleus (A,Z) can be calculated quite accurately using Eqs. (3) and (5), respectively, provided the corresponding analog neutron and two-neutron separation energies are known experimentally. The required generalized Coulomb shifts $\Delta_{np}(A,Z)$ and $\Delta_{2n2p}(A,Z)$ are determined by averaging the measured $\Delta_{np}(A',Z)$ and $\Delta_{2n2p}(A',Z)$ over A'. This technique is appropriate whenever $\Delta_{np}(A',Z)$ can determined from data for at least one A'; this limits its usefulness to the sd and lower fp shells. For heavier systems it is necessary to resort to one of the previously used techniques, such as that proposed in Ref. [17], which requires only that the analog neutron and two-neutron separation energies be known experimentally and that the necessary Coulomb displacement energies are available.

A slightly modified version of the proposed technique is also possible. Since $\Delta_{np}(A,Z)$ is assumed to be constant, we may replace it with any value $\Delta_{np}(A',Z)$, such as for $A'=2Z$. Then, from Eq. (7) we have

$$\Delta_{2n2p}(A,Z)=\Delta_{np}(2Z,Z)+\Delta_{np}(2Z-2,Z-1).$$

This is equivalent to an equation suggested by Goldansky [31] for the calculation of diproton separation energies, namely

$$S_{2n}(A,A-Z)-S_{2p}(A,Z)=S_n(2Z,Z)-S_p(2Z,Z)+S_n(2Z-2,Z-1)-S_p(2Z-2,Z-1).$$

Thus, a calculation for ^{31}Ar for example, would require the measured two-neutron separation energy $S_{2n}(^{31}\mathrm{Al})$ and single-nucleon separation energies of the self-conjugate nuclei ^{36}Ar and ^{34}Cl, namely $S_n(^{36}\mathrm{Ar})$, $S_p(^{36}\mathrm{Ar})$, $S_n(^{34}\mathrm{Cl})$, and $S_p(^{34}\mathrm{Cl})$. In fact, the computation can be made even simpler by using the fact that to the same approximation the generalized Coulomb shift $\Delta_{2n2p}(A,Z)$ is constant and assuming

$$\Delta_{2n2p}(A,Z)=\Delta_{2n2p}(2Z,Z).$$

One can easily show that the right-hand side of this equation is nothing more than the difference in binding energies of the analog pair with $T_3=\pm 1$ and $A=2Z-2$. The calculation for ^{31}Ar therefore requires only $S_{2n}(^{31}\mathrm{Al})$ and the ground-state binding energies of ^{34}Ar and ^{34}S.

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