Predicted proton and two-proton decay energies for nuclei in the upper *fp* shell

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The stability of proton-rich nuclei with Z=31-42 is investigated using measured binding energies of the analog neutron-rich nuclei and Coulomb energy shifts deduced from a parametrization of measured Coulomb displacement energies in the same mass region. Predicted binding energies and separation energies for proton and two-proton decay are compared with experimental information and with previous calculations where these are available. The positions of the one-proton and diproton drip lines are determined from the computed decay energies. Additional nuclides predicted to be proton stable but unstable to two-proton emission include several isotopes of Sr, Zr, and Mo. [S0556-2813(99)02802-2]

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I. INTRODUCTION

Diproton decay, the correlated emission of two protons, was first proposed as a possible exotic decay mode for proton-rich nuclei three decades ago by Goldansky [1]; the nucleon-nucleon pairing interaction in nuclei produces an even-odd staggering of proton separation energies, inhibiting proton emission for even Z nuclei near the driplines but having little effect on two-proton decay probabilities. Recent and ongoing experimental developments in radioactive-beam technology have brought the possibility of observable diproton decay closer to reality. In addition, several related calculational techniques have recently been proposed [2-7] which attempt to predict the proton and diproton separation energies of proton-rich nuclei with sufficient accuracy that candidates for observable diproton decay can be suggested. As a result of this work several candidates for diproton decay have been identified in the mass range $22 \le A \le 70$. The aim of the calculations reported here is to extend these predictions to $A \approx 80$, since this has become a region of considerable experimental activity in the last year or so [8-11]; in addition further information on proton-rich nuclides in this mass region is needed for a full understanding of astrophysical rp-processes of nucleosynthesis beyond nickel [12].

We use the method first proposed in Ref. [4]; the difference in ground-state binding energy between a proton-rich nucleus and the corresponding neutron-rich member of the same isospin multiplet is computed directly from the difference in Coulomb energies of the two nuclei. The Coulomb energies are determined using a method based on a parametrization of Coulomb displacement energies [13] for nuclei in a fixed model space. This technique was applied to nuclei at the interface between the *sd* shell and *fp* shell in Ref. [4] and to the complete *sd* shell in Ref. [7]. As a result of the calculations reported here, we are able to suggest several additional nuclides worthy of further study.

II. METHOD OF CALCULATION

Calculational details can be found in Refs. [4,7]; here we provide a brief summary. Consider a nucleus with Z active protons and N active neutrons in a suitable model space. The Coulomb energy of the nucleus, relative to the appropriate

inert core, can be expressed [13] as

$$E_{C}(Z,N) = Z\varepsilon_{C} + \frac{1}{2}Z(Z-1)V_{C} + \left[\frac{1}{2}Z\right]b_{C} + ZN\Delta_{np},$$
(1)

where $\left[\frac{1}{2}Z\right]$ indicates the largest integer not exceeding $\frac{1}{2}Z$, and ε_C , V_C and b_C are the Coulomb parts of the singleparticle energy, the average two-body matrix element and the pairing energy, respectively. The final term in Eq. (1) parametrizes in the simplest possible way the observed N dependence of Coulomb displacement energies for a chain of isotopes. We define the Coulomb displacement energy $\Delta^C(Z,N)$ as the total difference in binding energy between a given parent state and its isobaric analog; hence, from Eq. (1), we have

$$\Delta^{C}(Z,N) = \varepsilon_{C} + Z V_{C} + \delta(Z,\text{odd}) b_{C} + (N-Z-1)\Delta_{np},$$
(2)

where the quantity $\delta(Z, \text{odd})$ is unity if Z is odd and zero otherwise.

We assume that the ground-state binding energies of a proton-rich nucleus and the corresponding analog neutronrich nucleus differ only in their Coulomb energy contributions, i.e., we have

$$B(A,T,T_3 = -T) = B(A,T,T_3 = T) - \Delta E_C(A,T), \quad (3)$$

where A=N+Z is the number of valence nucleons, $T_3 = (N-Z)/2$ and $\Delta E_C(A,T)$, the Coulomb energy shift, is the difference in the Coulomb energies of the mirror pair. From Eq. (1) we have

$$\Delta E_{C}(A,T) = 2T \varepsilon_{C} + T (A-1) V_{C} + \left\{ T - \frac{1}{2} (-1)^{A/2 - T} \delta(2T, \text{odd}) \right\} b_{C}. \quad (4)$$

Within the same model, the proton separation energy of a proton-rich nucleus (A,T, -T) may be expressed in terms of the neutron separation energy of the analog neutron-rich nucleus (A,T,T) and a difference in Coulomb energy shifts:

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$$S_p(A,T,T_3=-T) = S_n(A,T,T_3=T) - D_1(A,T),$$
 (5)

where $D_1(A,T)$ is most conveniently expressed in terms of *Z* for the proton-rich nucleus:

$$D_1(A,T) = \varepsilon_C + (Z-1)V_C + \delta(Z, \text{even})b_C.$$
 (6)

Similarly, the separation energy for two-proton emission is

$$S_{2p}(A,T,T_3=-T) = S_{2n}(A,T,T_3=T) - D_2(A,T), \quad (7)$$

where

$$D_2(A,T) = 2\varepsilon_C + (2Z - 3)V_C + b_C.$$
(8)

Separation energies can also be computed as the difference in two binding energies, rather than using Eqs. (5) and (7). However, a major advantage in the present method, which produces explicit formulas for separation energies, is that the uncertainty in these quantities is thereby greatly reduced.

Implicit in the present method (and also in the methods of Refs. [2,3,6]) is the assumption that the nuclear wave functions of mirror states are identical; consequently we do not take into account corrections to the Coulomb energy of dripline nuclei due to the weak binding of the excess protons and the consequent spreading of the single-particle wave functions to larger radii. The self-consistent calculations of Ref. [14] suggest that these corrections may become significant for nuclei far from stability. However, it is not clear to what extent this effect is actually absorbed into the parameters of the present model.

III. PREDICTED PROTON AND TWO-PROTON SEPARATION ENERGIES

In this work we are initially concerned with the particledecay properties of proton-rich nuclei with $29 \le Z \le 40$. We assume that ⁵⁶Ni is a doubly-magic nucleus with valence nucleons occupying the $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ orbitals, and we proceed as follows. First, the four parameters of the model of Coulomb energies are determined by fitting measured displacement energies [15] for suitable parent-analog pairs with $29 \le (Z,N) \le 40$. In contrast to our previous work, we ignore any subshell dependence of the model parameters so that the one-orbital version of the model, Eq. (2), is sufficient; there is evidently significant configuration mixing, even for ground states, in this mass region, so that this approach is more realistic. Parameter values extracted from the fit are displayed as set 1 in Table I; the quantities in parentheses are uncertainties in the fit parameters. The smallness of these uncertainties and the standard deviation, σ =30 keV, suggests that Coulomb energies may well be accurately predicted by Eq. (1) using the parameters determined here. It should however be remembered that the data used to determine these parameters are exclusively for neutron-rich nuclei.

We now calculate, using Eqs. (3)-(8), binding energies and one- and two-proton separation energies for proton-rich nuclei with Z=31-40; the results are presented in Table II. The required properties of neutron-rich analog states are extracted from the compilation of Ref. [16], with recent data for A=80 from Ref. [11]. The quoted uncertainties reflect the uncertainties in both the data for analog states and the

TABLE I. Values of the parameters that define the Coulomb energy, determined from fits to Coulomb displacement energies. All energies are in keV and uncertainties are shown in parentheses. The number of data and the standard deviation are also shown. Set 1 and set 2 are the results of fits to two different data sets, as explained in the text.

Parameter	Set 1	Set 2	
ε _C	9582(13)	9504(17)	
V _C	226(7)	228(2)	
b_{C}	49(13)	30(12)	
Δ_{np}	-47(2)	-36(2)	
N	25	32	
σ	30	42	

Coulomb energy parameters; the latter is approximately proportional to the isospin *T*, whereas the former tends to be large for nuclei closest to N=Z. We include in the table nuclei up to and just beyond the proton and two-proton driplines; unfortunately it is impossible to make full predictions for a few nuclei with small isospin *T*, because of the lack of mass measurements for some N=Z nuclei and a few nuclei which are slightly neutron rich. We also include predicted particle separation energies for the interesting cases ⁵⁸Ga, ⁵⁸Ge, and ⁵⁹Ge, although these nuclei are outside the model space used to determine the Coulomb parameters; for these nuclei predicted binding energies are not included since these are more sensitive to uncertainties in the parameters.

Clearly, from Table II, there are many nuclei that are bound or quasibound to proton decay but unbound to twoproton emission in the ground state, especially for the larger values of Z. It therefore seems desirable to extend the calculations to heavier nuclei. However, for such nuclei configurations involving the $1g_{9/2}$ and $2d_{5/2}$ orbitals become increasingly important, and data dominated by these configurations were excluded from the fit to Coulomb displacement energies. In order to provide predictions for heavier nuclei we have therefore extracted a more appropriate set of Coulomb parameters. Using Eq. (2) we have analyzed all available data for ground states with $28 \le Z \le 42$ and $32 \le N \le 50$, irrespective of spin, parity, or configuration (three data were badly described and omitted from the final fit). The resulting Coulomb parameters are listed as set 2 in Table I and the predicted separation energies for Z=41 and 42 are shown in Table II. Use of the parameters of set 1 rather than set 2 would decrease S_p by 43 keV and 41 keV for isotopes of Nb and Mo, respectively, and the predictions for S_{2p} would be reduced by 110 keV and 104 keV.

No mass measurement exists for any proton-rich nucleus with Z>30, so that no comparison with experimental data is possible in this mass region. However, the nuclear mass compilation of Refs. [16] lists binding energies estimated from "systematic trends." The resulting separation energies differ significantly from the predictions in Table II, by about 200 keV on average, with no obvious systematic deviations.

Ormand [6] has recently calculated binding and separation energies for proton-rich nuclei with Z=25-36 using a technique that is also based on Eq. (1): Coulomb energy differences were calculated within the framework of the

TABLE II. Predicted binding energies (BE), proton separation energies (S_p) and two-proton separation energies (S_{2p}) for proton rich nuclei. All energies are in MeV and uncertainties are shown in parentheses. Calculations for isotopes of Nb and Mo are based on parameter set 2 of Table I; for the remaining nuclei, set 1 was used. Also included are the spin and parity of the analog ground state.

Nucleus	J^{π}	Т	Analog	BE	S_p	S_{2p}
⁵⁸ Ga	2^{+}	2	Co		-1.460(19)	0.058(36)
⁵⁹ Ga	$3/2^{-}$	3/2	Ni	485.980(47)	-1.034(19)	1.327(36)
⁶⁰ Ga	2^{+}	1	Cu	500.041(36)	0.028(19)	2.933(36)
⁶¹ Ga	$3/2^{-}$	1/2	Zn	515.190(25)	0.198(27)	5.337(54)
⁵⁸ Ge	0+	3	Fe		-0.264(28)	-2.651(46)
⁵⁹ Ge	$7/2^{-}$	5/2	Co		0.146(28)	-1.314(46)
⁶⁰ Ge	0^{+}	2	Ni	487.061(73)	1.080(28)	0.047(46)
⁶¹ Ge	3/2-	3/2	Cu	501.444(64)	1.402(28)	1.430(46)
⁶² Ge	0^{+}	1	Zn	517.778(47)	2.588(34)	2.786(49)
⁶³ Ge	3/2-	1/2	Ga	530.622(104)	2.456(104)	5.400(105)
⁶² As	1+	2	Cu	499.845(93)	-1.598(32)	-0.196(58)
⁰³ As	3/2-	3/2	Zn	516.406(77)	-1.371(33)	1.218(60)
⁶⁴ As	0+	1	Ga	530.354(58)	-0.267(105)	2.189(64)
⁶³ As	3/2	1/2	Ge	545.526(105)	-0.427(272)	4.596(145)
⁶² Se	0	3	N1	484.235(139)	-0.162(40)	-2.826(71)
⁶⁵ Se	3/2	5/2	Cu	499.939(132)	0.094(40)	-1.504(71)
⁶⁵ C	0^{+}	2	Zn	517.509(116)	1.103(40)	-0.268(71)
⁶⁶ Se	3/2	3/2	Ga	531.485(98)	1.131(40)	0.863(122)
67 S a	0 · 5/2 -	1/2	Ge	548.047(77)	2.525(108)	2.090(200)
66 D	$\frac{3/2}{0^+}$	1/2	AS Ca	500.841(108) 520.680(142)	1.000(123) - 1.705(45)	4.830(147) -0.665(84)
67 D #	$\frac{0}{1/2^{-}}$	2/2	Ga	529.009(142) 546.218(115)	-1.793(43) -1.921(54)	-0.003(84)
^{68}Br	1/2 3 ⁺	5/2	As	560 216(113)	-0.630(147)	1.092(131)
⁶⁹ Br	3/2-	1/2	A5 Se	575 685(54)	0.030(147)	1.234(142)
⁶⁶ Kr	0^{+}	3	Zn	$514\ 403(212)$	-0.150(53)	-3.106(98)
⁶⁷ Kr	3/2-	5/2	Ga	529 705(195)	0.017(53)	-1.779(98)
⁶⁸ Kr	0^{+}	2	Ge	547 403(168)	1.185(54)	-0.647(102)
⁶⁹ Kr	5/2-	3/2	As	561.276(140)	1.065(113)	0.435(143)
⁷⁰ Rb	4+	2	As	559.230(201)	-2.055(84)	-0.990(156)
⁷¹ Rb	5/2-	3/2	Se	576.397(200)		0.713(171)
⁷² Rb	3+	1	Br	590.314(283)		
⁷³ Rb	$5/2^{-}$	1/2	Kr	606.544(152)	-0.542(306)	
⁷⁰ Sr	0^{+}	3	Ge	544.082(293)	-0.123(67)	-3.321(125)
⁷¹ Sr	$5/2^{-}$	5/2	As	559.187(262)	-0.038(84)	-2.093(129)
⁷² Sr	0^{+}	2	Se	577.238(223)	0.840(142)	
⁷³ Sr	$1/2^{-}$	3/2	Br	591.103(221)	0.790(232)	
⁷⁴ Sr	0^{+}	1	Kr	608.233(139)	1.695(164)	1.152(302)
⁷⁵ Sr	$(3/2, 5/2)^{-}$	1/2	Sr	621.964(68)	1.907(723)	4.037(155)
⁷⁴ Y	(0 ⁻)	2	Br	589.107(251)	-1.992(149)	-1.202(295)
⁷⁵ Y	$(5/2)^+$	3/2	Kr	606.542(198)	-1.694(94)	0.001(197)
⁷⁰ Y	1(-)	1	Rb	621.456(139)	-0.508(74)	1.400(733)
//Y	$(5/2^+, 3/2^+)$	1/2	Sr	637.903(167)	()	4.278(167)
⁷⁴ Zr	0	3	Se	573.749(376)	-0.044(82)	-3.488(154)
⁷⁵ Zr	3/2	5/2	Br	588.900(331)	-0.208(83)	-2.200(204)
70 Zr	0^{+}	2	Kr	607.239(278)	0.696(82)	-0.99/(164)
78 Z	3/2	3/2	Rb	621.761(220)	0.305(82)	-0.203(153)
⁷⁹ 7 ⁿ	$(5/2^+)$	1/2	Sr	639.039(133)	1.159(170)	2621(491)
78NIL	(3/2)	1/2	I Dh	035.508(457)	-2.064(28)	5.031(461) - 1.602(52)
⁷⁹ Nb	$\frac{0}{3/2}(-)$	2/2	KU Sr		-2.004(28) -1.871(28)	-0.645(160)
⁸⁰ Nb	(3.1.5)	J/∠ 1	V		-1.345(481)	0.045(100)
⁸¹ Nb	(3,4,3)	1/2	T Zr		-800(1520)	3 614(540)
⁷⁸ Mo	0^+	3	Kr		-0.443(30)	-3473(54)
⁷⁹ Mo	5/2+	5/2	Rh		-0.571(31)	-2.634(55)
⁸⁰ Mo	0^{+}	2	Sr		0.396(31)	-1.474(55)
⁸¹ Mo	$(5/2^+)$	3/2	Y		0.400(180)	-0.946(457)
⁸² Mo	0^{+}	1	Zr		0.905(591)	0.110(1580)
⁸³ Mo	(5/2+)	1/2	Nb			2.962(434)

nuclear shell model using an effective Coulomb plus isovector and isotensor interaction. Direct comparison is therefore possible between Ormand's predictions for Z=31-36 and the present work. For isotopes of Ge, Ga, As, and Se the agreement is impressive, with an average difference in energy of less than 40 keV. However, for isotopes of Br and Kr Ormand's predictions¹ for binding energies and separation energies are systematically more positive, by 150 keV on average. Much better agreement between the two calculations is achieved for isotopes of Br and Kr if parameter set 2 is employed rather than set 1 (S_p is increased by 61 and 78 keV and S_{2n} by 144 and 138 keV, respectively); however the agreement for lighter systems becomes worse. Possibly parameter set 2 is more appropriate for all nuclei with $Z \ge 35$. Note that the quoted uncertainties are always smaller in the present work, often substantially smaller, for the reason mentioned above.

In the past few years there have been a number of studies of proton-rich nuclei using various self-consistent mean-field theories. Ground-state binding energies have also been computed using various mass formulas; one sophisticated variant is the microscopic-macroscopic model developed by Möller and co-workers [18]. Although both these approaches give a reasonable global description of nuclear binding energies (and other nuclear properties), their usefulness in predicting reliable particle-decay lifetimes is more limited. As an example, relativistic mean-field calculations for even-even proton-rich nuclei with $10 \le Z \le 82$ have recently been reported [17]. In the four cases where comparison is possible, the predicted two-proton separation energies of Ref. [17] are more negative than those reported here by up to 1.8 MeV; differences of this magnitude produce different driplines and partial decay lifetimes which differ by many orders of magnitude.

IV. SUMMARY AND CONCLUSION

The primary purpose of this work is to determine the proton and diproton driplines for fp-shell nuclei, and to suggest candidates for observable diproton decay. To determine the actual decay mode of these nuclei one needs to know their partial lifetimes for all possible decay processes. Those for β^+ decay and electron capture can only be determined from more detailed structure calculations; however, as Ormand [3] has pointed out, the β -decay lifetimes will be short (they are of the order 10 ms for light fp-shell dripline nuclei) since the β^+ -decay end-point energies are large. Partial lifetimes for particle emission are determined mainly by proton and diproton penetrability factors, which depend on the angular momentum of the emitted particle (zero for correlated diproton emission), the mass number of the emitter and, with extreme sensitivity, on the separation energy of the emitted particle.

The positions of the particle driplines can in most cases be deduced from the information in Table II, although a few additional comments are necessary. The N=Z nuclei ⁶⁶As and ⁷⁴Rb are known experimentally to be bound to proton emission and are therefore at the proton dripline. Lack of mass measurements for the N=Z nuclei ⁶⁸Se, ⁷⁶Sr, ⁷⁸Y, and ⁸⁰Zr prevents the unambiguous prediction of the proton dripline for Br and Y and the diproton dripline for Sr, Zr, Nb, and Mo. However, the masses derived from systematic trends in Ref. [16] suggest that ⁶⁹Br and ⁷⁷Y are beyond the proton dripline, whereas ⁷⁸Y is proton stable; there is also experimental evidence from lifetimes that ⁶⁹Br and ⁷⁷Y are proton unbound [9,19]. In fact, recent experiments [9,10] on $T_3 = -1/2$ nuclei suggest that ⁷⁵Sr, ⁷⁹Zr, and ⁸³Mo are particle stable, whereas ⁶⁹Br, ⁷³Rb, and ⁸¹Nb decay by particle emission; the predictions presented in Table II are consistent with these experiments. Lack of experimental information for neutron-rich nuclei also prevents the determination of the position of the two-proton dripline for isotopes of Sr; the two-proton separation energy of ⁷³Sr deduced from systematic trends in Ref. [16] is consistent with zero. Finally, the $T_3 = -1$ nuclei ⁷⁸Zr, ⁸⁰Nb, and ⁸²Mo are almost certainly stable against diproton emission.

In Ref. [6] partial decay lifetimes are estimated for several potential diproton emitters in this mass region using the WKB approximation for the partial decay width. Ormand [6] has estimated that, in order to be observable, the diproton half-life must be in the approximate range $10^{-8} - 10^{-3}$ s; this ensures that the decaying nucleus will live long enough to be identified and that this decay mode can compete with β decay. Using this criterion and Ormand's calculated separation energies, ⁵⁹Ge, ⁶³Se, and ⁶⁷Kr were identified as the best candidates for observable diproton decay amongst nuclei with Z = 31 - 36. Use of the separation energies reported in Table II reinforces this conclusion; in fact, ⁶⁷Kr is predicted to be an ideal candidate since the separation energy is reduced somewhat in this work (by 100 keV using parameter set 2), pushing the predicted lifetime further in to the observable range. Of the nuclei not considered in Ormand's study, ⁷¹Sr probably has a lifetime that is too short for observation; the separation energy of ⁷²Sr could not be calculated, but the lifetime for diproton decay may well fall in the correct range. Similarly, the diproton lifetime of ⁷⁵Zr may be too short for observation whereas that of ⁷⁶Zr is probably too long, so that its primary decay mode will be β^+ . Finally, of the Mo isotopes, ⁸⁰Mo and ⁸¹Mo are possible candidates for observable diproton radioactivity, although a more accurate mass estimate is required in the latter case.

¹The predicted binding energy tabulated in Ref. [6] for ⁶⁹Kr is not consistent with the listed separation energies involving this nucleus; the discrepancy is 1.037 MeV. We have assumed that the binding energy is correct. This implies that Ormand's conclusions regarding this nucleus require modification.

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