MASTER

Construction of an Extended Nuclidic Mass Table*

by

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CONF-52-4

The calculation of cross sections of high energy nuclear reactions requires a fairly accurate table of masses of a large number of unknown nuclides. The best extended nuclidic mass table (1) (at the time this work began) included quite a few with deviations between known and calculated masses greater than 1 MeV and ranging up to 6 MeV. Such discrepancies naturally cause one to be suspicious about the values calculated for unknown masses. The following report describes an attempt to construct an extended mass table with very small deviations among the known masses. It is based on a re-examination (2,3,4) of "parabolic systematics".

The Weizacker(5) mass formula is parabolic in Z at constant A . Changing (1) the Coulomb term to trapezoidal charge distribution introduces a $Z^{4/3}$ term; however, this latter term will be ignored for the time being. When expressed in the form

$$\Delta M = a + bZ + cZ^2$$

*This work was performed under the auspices of the U. S. Atomic Energy Commission.

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the determination of the parameters a, b, and c versus A would allow the use of this formula for the calculation of unknown masses. The parameters, and their products with powers of Z are very much larger than the excess masses themselves, requiring their knowledge to a large number (~5) of significant figures to obtain meaningful results. Translation of the axis to the symmetry line transforms the equation to

$$\Delta M = A_0 + B(Z-Z_0)^2 + \delta$$

where A_0 is the minimum excess mass, Z_0 is the charge at the minimum, and B is the curvature of the parabola. The δ term is introduced to accommodate pairing corrections. The formula in this form has been discussed previously (3,4). For use, the parameters do not require a large number of significant figures.

There is sufficient data in the 1961 Mass Table (6) to determine the parameters for 149 of the 382 parabolas (two for each even A) for isobars 1 through 255. By means of further considerations this may be improved considerably. The values for Z_0 and A_0 fall as illustrated in Figures 1 and 2. Only a very insignificant difference could be discerned for Z_0 for parabolas of odd-odd and even-even nuclides of the same isobar, and the values were accepted as identical. For even-A isobars values of A_0 are plotted separately for the parabolas of odd-odd (crosses) and even-even (circles) nuclides.

No attempt was made to fit these curves to any formula. Instead a parabolic interpolation procedure was used to determine the missing points. The interpolation procedure was evaluated by determining known values by the same method. The check was quite good. The δ 's were then determined as the difference of known A_0 's for the even-A isobars and the values of the A_0 's for even-A isobars as determined by interpolation of the A_0 's for odd-A isobars (Figure 3). Fitting the δ 's to an apparent straight line allowed a reasonable estimation of the remaining even-A A_0 's.

The entire problem can be simplified by an elementary consideration of the two parabolas at even-A isobars. They may not cross. For if they did, this would result in positron emission on the neutron excess side and negatron emission on the proton-rich side. Consequently the curvature, B , for the odd-odd parabola must be either greater than or equal to the curvature of the even-even parabola. The curvatures of most of the parabolas can be determined from the mass data and from the interpolated values of Z_0 and A_0 . It appears from the data, that except at low A , the calculated curvatures of the odd-odd nuclide parabolas are scattered both higher and lower than the curvatures of the corresponding even-even nuclide parabolas. The curvatures of both parabolas were then assumed to be equal.

This consideration, therefore, reduces the number of parabolas to 255 and increases the number for which parameters are directly determinable to 229. The rest were determined by means of the interpolation procedure for missing Z_0 's and A_0 's and using the estimated linear relationship for the δ 's. No interpolation procedure was possible for B since the values were too scattered (Figure 4). A few still indeterminable in this way required the use of additional data from the Nuclear Data Sheets.

The mass table constructed from these parameters is, on the surface, excellent. The standard deviation is 0.255 and there are only 8 deviations greater than 1 MeV. (For comparison with other tables only isobars of A greater than 21 were considered). There is, however, a very serious flaw. For many isobars, the Q for neutron emission is positive on the proton-rich side and/or negative on the neutron-rich side. The case is similar for proton emission. In order to alleviate this fault one must invoke some of the properties of the systematics of the binding energies of protons, neutrons and alpha particles.

When considering proton and/or neutron decay systematics, one ordinarily expects that a nuclide of all protons or all neutrons should spontaneously emit protons or neutrons respectively, while nuclides containing only one proton or neutron should not spontaneously emit those respective particles.

Generally, for spontaneous particle emission

$$\Delta M_i > \Delta M_f + \Delta M_p.$$

For non-emission the sign is reversed. Thus, for example, for non-neutron emission

$Ao_i + B_i (Z_j - Zo_i)^2 + \delta_i < Ao_{i-1} + B_{i-1} (Z_j - Zo_{i-1})^2 + \delta_{i-1} + n$,
and, since in the extreme cases the charge of initial and final nuclides is $A_i - 1$, then

$$\frac{B_i}{B_{i-1}} < \frac{(A_i - 1 - Zo_{i-1})^2 + Ao_{i-1} - Ao_i + \delta_{i-1} - \delta_i + n}{(A_i - 1 - Zo_i)^2}.$$

Similarly, for spontaneous neutron emission

$$\frac{B_i}{B_{i-1}} > \frac{(Zo_{i-1})^2 + Ao_{i-1} - Ao_i + \delta_{i-1} - \delta_i + n}{(Zo_i)^2},$$

for non-proton emission

$$\frac{B_i}{B_{i-1}} < \frac{(Zo_{i-1})^2 + Ao_{i-1} - Ao_i + \delta_{i-1} - \delta_i + p}{(1 - Zo_i)^2},$$

and for spontaneous proton emission

$$\frac{B_i}{B_{i-1}} > \frac{(A_i - 1 - Zo_{i-1})^2 + Ao_{i-1} - Ao_i + \delta_{i-1} - \delta_i + p}{(A_i - Zo_i)^2}.$$

Both nuclides containing only two protons and nuclides having only two neutrons may not undergo spontaneous alpha emission.

For these,

$$\frac{B_i}{B_{i-1}} < \frac{(A_i - 4 - Zo_{i-4})^2 + Ao_{i-4} - Ao_i + \delta_{i-4} - \delta_i + \alpha}{(A_{i-2} - Zo_i)^2},$$

and

$$\frac{B_i}{B_{i-1}} < \frac{(Z_{o_{i-4}})^2 + A_{o_{i-4}} - A_{o_i} + \delta_{i-4} - \delta_i + \alpha}{(2 - Z_{o_i})^2} .$$

Thus, using predetermined values for Z_o and A_o , the maxima and minima relative curvatures for all isobars may be calculated. Based on the nonspontaneous neutron emission data, it appears that there may not be as much scatter in the curvatures as there appears to be in Figure 4. More significantly since the ratios $\frac{B_i}{B_{i-1}}$ for non-spontaneous proton-rich alpha-emission are almost all less than one, it appears, provided that the assumption of no alpha emission is correct, that, except for low A 's, the function of B versus A must be monotonically decreasing.

The choice of a monotonically decreasing function for B versus A should probably be governed by considerations of best fit. In Figure 4 the solid line is the curve for the relationship derivable from the Weizsacker Mass Formula,

$$B = a_3 A^{-1} + 3e^2 A^{-2/3} / 5r_0$$

with a_3 and r_0 as free parameters. These were determined from a least squares fit as 76.1 MeV and 1.32 Fermis respectively. An even better fit, especially in the $A = 40$ to 100 isobar region is obtainable by treating the function as a sum of two exponentials. This has no bearing on any theory that I am aware of but is tentatively useful.

Now that one parameter of the parabola, B , has a fixed form,

and its best values have been determined, the values of A_0 , Z_0 , and δ may be redetermined. Only two masses are required for each odd-A isobar and only three are required for each even-A isobar. Sufficient data is in the 1961 Mass Table to determine all of the parameters for 245 of the 255 parabolas. Only two of these are in the isobar region 13 through 246. The unknown parameters were determined by the interpolation procedure and an extended mass table* was constructed. Nineteen calculated masses deviated from the known masses by more than one MeV. All but one were associated with closed-shell effects, for which no correction at all has been made. The largest deviation is 2.0 MeV and the standard deviation for 763 masses was 0.35 MeV. Certainly further refinements are possible.

*The mass table will be available as a Brookhaven National Laboratory report.

References

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Figures

Figure 1 - Z_0 vs. A . Data obtained from odd- A isobars with more than three masses available and from even- A isobars with more than three masses of even-even and/or more than three masses of odd-odd nuclides available.

Figure 2 - A_0 vs. A . Data obtained as in Figure 1. $\odot$ - odd- A isobars; $\circ$ - even- A isobars, even-even nuclides; $\times$ - even- A isobars, odd-odd nuclides.

Figure 3 - δ vs. A . $\odot$ - even-even nuclides; $\boxtimes$ - odd-odd nuclides.

Figure 4 - B vs. A . $\odot$ - odd- A isobars, $\circ$ - even- A isobars.

Solid curve represents the fit of the data to

$$B = aA^{-1} + bA^{-1/3}.$$