Relations for the coefficients in the $I(I+1)$ expansion for rotational spectra

F. X. Xu
Department of Physics, Anhui University, Hefei, China

C. S. Wu and J. Y. Zeng
Department of Physics, Peking University, Beijing, China
and China Center of Advanced Science and Technology (World Laboratory),
Center of Theoretical Physics, Beijing, China
(Received 29 June 1989)

All the data now available for the ground rotational bands of actinide even-even nuclei and of rare-earth even-even nuclei (with bandcrossing angular momentum $I_c \geq 16$) are analyzed with the four-parameter $I(I+1)$ expansion. The parameters obtained by the least-squares fitting definitely deviate from the relations derived from the Harris two-parameter ω^2 expansion, but are closer to the relations deduced from the closed two-parameter expression by Wu and Zeng.

On the basis of consideration of symmetry, Bohr and Mottelson pointed out[1] that for an axial symmetric nucleus the rotational energy E is a function of $I(I+1)$. For small values of I, E can be expanded in powers of $I(I+1)$. In particular, for the ground rotational band (GRB) of an even-even deformed nucleus

$$E(I)=AI(I+1)+B[I(I+1)]^2+C[I(I+1)]^3+D[I(I+1)]^4+\cdots \quad (1)$$

Harris suggested[2] that E may be expanded in powers of ω^2 instead of $I(I+1)$, namely

$$E=\alpha\omega^2+\beta\omega^4+\gamma\omega^6+\delta\omega^8+\cdots , \quad (2)$$

where ω is the angular frequency of rotation along the x axis. ω is not a directly observed quantity, but is derived from the observed rotational spectra according to the canonical relation[3]

$$\hbar\omega=\frac{dE}{dI_x}, \quad I_x=[(I+\tfrac{1}{2})^2-K^2]^{1/2} . \quad (3)$$

From the analysis of observed rotational spectra in the early seventies,[4] it is believed that the ω^2 expansion converges better than the $I(I+1)$ expansion. Mottelson pointed out[5] that if the expansion in ω^2 is more rapidly convergent than that in $I(I+1)$, we can exploit this fact to obtain relations between the higher coefficients in the $I(I+1)$ expansion. Particularly, including only two terms in Eq. (2), i.e.,

$$E=\alpha\omega^2+\beta\omega^4 \quad (4)$$

implies the relations[1]

$$\frac{C}{A}=4\left[\frac{B}{A}\right]^2, \quad \frac{D}{A}=24\left[\frac{B}{A}\right]^3 . \quad (5)$$

TABLE I. The A, B, C, and D values (in keV) for the GRB's of even actinide nuclei obtained by the least-squares fitting.

Nuclei	A	$B\times10^3$	$C\times10^6$	$D\times10^9$	$\frac{AC}{4B^2}$	$\frac{A^2D}{24B^3}$
^{248}Cm	7.2206	−2.681	0.858	0.03	0.215	−0.003
^{244}Pu	7.6529	−4.114	4.911	−3.94	0.555	0.138
^{242}Pu	7.4296	−3.540	3.369	−1.92	0.499	0.100
^{240}Pu	7.1620	−3.957	6.954	−9.42	0.795	0.325
^{238}Pu	7.3678	−3.670	5.747	−5.84	0.786	0.267
^{236}Pu	7.3537	−3.157	0.023	3.04	0.004	−0.218
^{238}U	7.4298	−3.736	2.471	−0.87	0.329	0.038
^{236}U	7.5122	−3.920	2.575	−0.80	0.315	0.031
^{234}U	7.2015	−4.710	4.428	−1.68	0.359	0.039
^{232}U	7.9245	−6.372	9.025	−6.90	0.440	0.070
^{230}U	8.6401	−9.772	20.786	−22.69	0.470	0.076
^{232}Th	8.1138	−6.080	5.819	−2.45	0.319	0.030
^{230}Th	8.7817	−8.219	11.519	−7.73	0.374	0.045
^{228}Th	9.6640	−17.975	60.803	−104.87	0.455	0.070

TABLE II. The A, B, C, and D values (in keV) for the GRB's of even rare-earth nuclei obtained by the least-squares fitting.

Nuclei	A	$B\times10^3$	$C\times10^6$	$D\times10^9$	$\frac{AC}{4B^2}$	$\frac{A^2D}{24B^3}$
^{178}Hf	15.5448	−11.844	2.752	5.28	0.076	−0.032
^{176}Hf	14.7758	−14.218	23.640	−24.77	0.432	0.078
^{174}Hf	15.1814	−17.617	23.996	−18.27	0.293	0.032
^{172}Hf	15.8490	−23.164	50.298	−60.70	0.371	0.051
^{170}Hf	16.7024	−37.103	102.343	−129.01	0.310	0.029
^{176}Yb	13.7152	−6.446	0.143	2.46	0.012	−0.072
^{174}Yb	12.7746	−6.337	6.639	−4.16	0.528	0.111
^{172}Yb	13.1565	−7.568	12.086	−11.66	0.694	0.194
^{170}Yb	14.0896	−11.242	24.103	−54.17	0.672	0.315
^{168}Yb	14.6797	−19.059	34.573	−37.56	0.349	0.049
^{166}Er	13.4801	−12.225	11.572	−4.83	0.261	0.020
^{164}Er	15.3073	−17.932	47.446	−82.60	0.565	0.140
^{164}Dy	12.2744	−8.499	11.584	−10.32	0.492	0.106
^{162}Dy	13.4412	−9.875	13.486	−10.56	0.465	0.083
^{156}Gd	14.8553	−24.998	77.901	−135.37	0.463	0.080

In Table 4-2 of Ref. 1, these relations were investigated with the observed data for ^{168}Er, ^{178}Hf, and ^{162}Gd for which sufficiently accurate energy measurements were available. It is found that the relations (5) are approximately obeyed. In the past decade, the cranked shell model (CSM) in its various versions were successfully used for the descriptions of high-spin nuclear states.[3] In the CSM formalism, the Harris two-parameter ω^2 expansion (4) and the corresponding expression for the kinematical moment of inertia

$$\mathcal{J}=\mathcal{J}_0+\mathcal{J}_1\omega^2(=2\alpha+\tfrac{4}{3}\beta\omega^2) \tag{6}$$

are widely used for the parametrization of data.

However, in most rare-earth nuclei, because of the crossing of the GRB by the S band at $I\approx10-12$, usually only 4–5 yrast levels ($I\leq10$) belong to the GRB. This clearly limits the conclusions that can be made about the applicability of (4) to the GRB. In recent years Coulomb excitation experiments with very heavy ion beams (e.g., ^{208}Pb ions) on the actinide nuclei have provided abundant information about the high-spin levels of actinide GRB's. Because the moments of inertia of actinide nuclei are about twice those of the rare-earth nuclei, the two-quasiparticle S band does not compete with the GRB until much higher spins. Therefore, the yrast levels with even spin and parity in actinide nuclei may belong to the GRB's with much higher spins than those in rare-earth nuclei. In fact, the only pronounced backbending known is in ^{244}Pu at $I\approx22$; and in ^{232}Th, ^{234,236,238}U, and ^{248}Cm no pronounced backbending has been observed up to $I\approx30$ ($\hbar\omega\approx270$ keV). Thus, the recent data provide an ideal opportunity to test the applicability of various for-

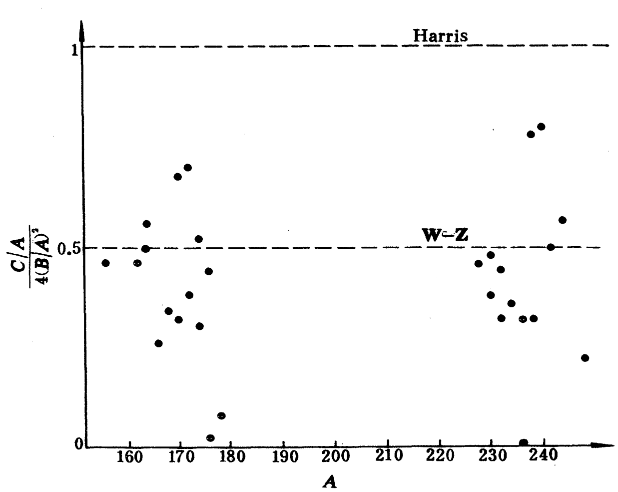

FIG. 1. $AC/4B^2$ vs A plot.

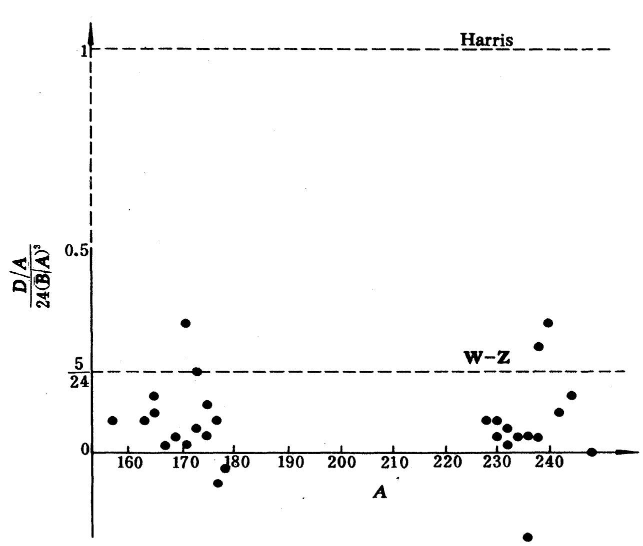

FIG. 2. $A^2D/24B^3$ vs A plot.

TABLE III. Experimental and calculated energies (in keV) of the GRB's of even actinide nuclei. The calculated values correspond to the four-parameter $I(I+1)$ expansion (1). The values of A, B, C, and D are listed in Table I. σ is the root-mean-square deviation defined by Eq. (9).

Nuclei	$I=2$	4	6	8	10	12	14	16	18	20	22	24	26	28	σ
^{248}Cm Exp[a]	43.4	144.2	299.5	506.9	763.0	1064.0	1405.4	1782.8	2190.7	2624.6	3080.6	3556.0	4051.0	4567.3	
Cal	43.23	143.35	298.60	506.31	762.98	1064.45	1406.10	1783.08	2190.58	2624.17	3080.20	3556.20	4051.36	4567.13	0.481
^{244}Pu Exp[b]	46.1	152.3	314.7	531.1	797.6	1110.1	1463.7	1854.7	2278.5	2730.0					
Cal	45.77	151.45	314.52	531.41	798.00	1110.05	1463.52	1854.52	2278.74	2729.94					0.353
^{242}Pu Exp[c]	44.54	147.3	306.4	518.1	778.7	1084.0	1431.3	1816.3	2235.6	2686.0	3163	3662			
Cal	44.45	147.20	306.04	517.79	778.62	1084.52	1431.56	1816.22	2235.32	2685.74	3163.43	3661.87			0.279
^{240}Pu Exp[d]	42.83	141.69	294.32	497.50	747.8	1041.8	1375.6								
Cal	42.83	141.71	294.31	497.49	747.81	1041.79	1375.60								0.011
^{238}Pu Exp[d]	44.08	145.98	303.4	513.4	772.8	1078.5	1427.2	1816.2	2240.5						
Cal	44.08	145.93	303.38	513.44	772.84	1078.42	1427.25	1816.19	2240.50						0.041
^{236}Pu Exp[d]	44.63	145	303.5	513.4	771.2	1072.0	1411.3	1783.7							
Cal	44.01	145.81	303.30	513.19	771.18	1072.23	1411.17	1783.72							0.388
^{238}U Exp[e]	44.91	148.41	307.21	517.8	775.7	1076.5	1415.3	1788.2	2190.7	2618.7	3067.2	3534.5	4017.3	4516.5	
Cal	44.44	147.12	305.64	516.47	775.23	1076.98	1416.67	1789.44	2190.95	2617.52	3066.16	3534.25	4018.91	4515.89	1.055
^{236}U Exp[f]	45.24	149.48	309.79	522.25	782.8	1086.2	1425	1800	2203	2630	3080	3549	4038	4548	
Cal	44.93	148.70	308.79	521.50	782.22	1085.81	1426.98	1800.75	2202.76	2629.60	3078.86	3549.04	4039.09	4547.57	0.852
^{234}U Exp[g]	43.48	143.34	296.04	497.02	741.2	1024.0	1340.8	1688.0	2063.0	2464.2	2889.7	3339	3808	4297	
Cal	43.04	142.18	294.48	495.69	740.79	1024.50	1341.94	1689.15	2063.41	2463.36	2888.52	3338.28	3810.03	4296.29	1.077
^{232}U Exp[h]	47.57	156.17	322.3	540.7	805.5	1111.2	1453.5	1828.0	2231.5	2658.4					
Cal	47.32	156.01	322.24	540.72	805.60	1111.35	1453.33	1827.94	2231.60	2658.37					0.129
^{230}U Exp[d]	51.72	169.5	347.0	578.3	856.5	1175.8	1531.7	1921.3							
Cal	51.49	169.06	347.12	578.58	856.52	1175.53	1531.87	1921.27							0.235
^{232}Th Exp[e]	49.37	162.12	333.2	556.9	827.0	1137.4	1482.8	1858.9	2262.9	2691.9	3144.9	3619.0	4116.9	4632.9	
Cal	48.47	159.89	330.48	554.78	826.34	1138.43	1484.91	1860.86	2263.11	2690.34	3142.51	3619.54	4118.93	4632.03	1.708
^{230}Th Exp[e]	53.20	174.06	356.6	594.1	879.7	1207.8	1572.9	1971.5	2397.8	2850	3325				
Cal	52.40	172.44	355.16	593.77	880.74	1209.09	1573.35	1970.05	2397.04	2851.32	3324.63				1.088
^{228}Th Exp[i]	57.76	186.82	378.17	622.2	911.5	1238.7	1595.9								
Cal	57.35	186.56	378.36	622.50	911.12	1238.86	1595.87								0.277

[a]References 9 and 10.
[b]Reference 11.
[c]Reference 12.
[d]Reference 13.
[e]Reference 14.
[f]Reference 15.
[g]Reference 16.
[h]Reference 17.
[i]Reference 18.

mulas for rotational spectra.

In Refs. 6 and 7 the collective spectra of a well-deformed nucleus with a small axial asymmetry ($\sin^2 3\gamma \ll 1$) are investigated in the framework of Bohr Hamiltonian. The rotational energy is expanded in powers of $\sin^2 3\gamma$ and the terms of $\mathcal{O}(\sin^4 3\gamma)$ are neglected. When a suitable β separable potential is adopted, a very simple two-parameter expression for the rotational band is obtained, and for the GRB of an even-even nucleus it reads

$$E(I)=a\{[1+bI(I+1)]^{1/2}-1\} . \tag{7}$$

It is found that such a simple formula can fit the observed rotational spectra very well up to very high spins.[8] Expanding Eq. (7) in powers of $I(I+1)$, one can easily verify that

$$\frac{AC}{4B^2}=\frac{1}{2}, \quad \frac{A^2D}{24B^3}=\frac{5}{24} , \tag{8}$$

which is quite different from the relations (5) obtained by Harris two-parameter expression (4).

In this paper, all the data now available for the GRB's of actinide even-even nuclei and of some rare-earth nuclei (which have bandcrossing angular momentum $I_c \geq 16$) are analyzed with the four-parameter $I(I+1)$ expansion (1). The coefficients A, B, C, and D obtained by the least-squares fitting are listed in Tables I and II. The calculated energy spectra with these parameters are compared with the observed GRB's in Tables III and IV. The $AC/4B^2$ vs A and $A^2D/24B^3$ vs A plots are shown in Figs. 1 and 2.

It can be seen from Tables III and IV that the four-parameter $I(I+1)$ expansion (1) can fit the GRB's (below bandcrossing) of well-deformed nuclei very well. In most nuclei the root-mean-square deviations

$$\sigma=\left[\frac{1}{N}\sum_{i=1}^{N}|(E_{\text{cal}}-E_{\text{exp}})_i|^2\right]^{1/2} \tag{9}$$

are very small. Therefore, in contrast to the usual im-

TABLE IV. Experimental and calculated energies (in keV) of the GRB's of even rare-earth nuclei. The calculated values correspond to the four-parameter $I(I+1)$ expansion (1). The values of A, B, C, and D are listed in Table II.

Nuclei	$I=2$	4	6	8	10	12	14	16	18	20	σ
^{178}Hf Exp[a]	93.17	306.61	632.2	1058.6	1571.0	2150.7	2777.6	3436.2			
Cal	92.84	306.18	632.21	1059.00	1571.05	2150.32	2777.82	3436.16			0.284
^{176}Hf Exp[b]	88.36	290.19	597.08	998.1	1481.4	2034.0	2646.7				
Cal	88.15	290.01	597.18	998.31	1481.15	2034.11	2646.68				0.172
^{174}Hf Exp[c]	90.99	297.38	608.3	1009.6	1485.9	2020.5	2597.5	3208.9			
Cal	90.46	296.77	608.26	1010.20	1486.05	2019.85	2597.87	3208.83			0.448
^{172}Hf Exp[d]	95.24	309.26	628.1	1037.3	1521.1	2064.6	2654.0	3277.2			
Cal	94.27	308.11	628.33	1038.19	1521.17	2063.73	2654.52	3277.10			0.721
^{170}Hf Exp[e]	100.80	321.99	642.9	1043.3	1505.5	2016.4	2567.2	3151.6			
Cal	98.90	320.00	643.23	1044.96	1505.65	2014.77	2568.17	3151.42			0.327
^{176}Yb Exp[a]	82.13	271.69	564.8	954.1	1431.2	1984.8	2602	3270			
Cal	82.06	271.73	564.69	954.20	1431.23	1984.71	2602.05	3269.99			0.071
^{174}Yb Exp[c]	76.47	253.12	526.04	889.9	1336	1861	2457	3117	3836	4610	
Cal	76.42	253.01	525.83	889.29	1336.75	1861.36	2456.59	3116.68	3836.37	4609.91	0.393
^{172}Yb Exp[d]	78.75	260.29	540.00	912.2	1370.1	1907.2	2518.4	3198.1			
Cal	78.67	260.20	540.08	912.24	1370.03	1907.23	2518.40	3198.10			0.061
^{170}Yb Exp[e]	84.26	277.45	573.54	963.7	1438.0	1983.8	2580.9				
Cal	84.14	277.48	573.55	963.71	1437.98	1983.81	2580.90				0.049
^{168}Yb Exp[a]	87.73	286.55	585.30	970.1	1424	1936	2489	3073			
Cal	87.40	286.24	585.37	970.03	1424.67	1935.22	2489.36	3072.94			0.419
^{166}Er Exp[f]	80.57	264.99	545.44	911.2	1349.6	1846.6	2389.4	2968.6			
Cal	80.44	264.80	545.44	911.38	1349.59	1846.47	2389.48	2968.58			0.117
^{164}Er Exp[g]	91.39	299.46	615.4	1024.6	1518.0	2082.7	2702.5				
Cal	91.21	299.34	614.53	1024.60	1517.88	2082.75	2702.49				0.110
^{164}Dy Exp[g]	73.39	242.23	501.32	843.7	1261.3	1745.8	2290				
Cal	73.34	242.16	501.36	843.74	1261.24	1745.82	2290.00				0.040
^{162}Dy Exp[h]	80.66	265.66	548.52	920.9	1374.9	1901.4	2492.4	3138.4	3837.0		
Cal	80.29	265.98	548.08	921.33	1375.45	1901.45	2491.52	3139.00	3836.88		0.519
^{156}Gd Exp[i]	88.97	288.18	584.71	965.1	1416.0	1924.4	2475.4				
Cal	88.25	287.71	585.17	965.43	1415.47	1924.64	2475.36				0.449

[a]Reference 14.
[b]Reference 19.
[c]Reference 20.
[d]Reference 21.
[e]Reference 22.
[f]Reference 23.
[g]Reference 24.
[h]Reference 25.
[i]Reference 26.

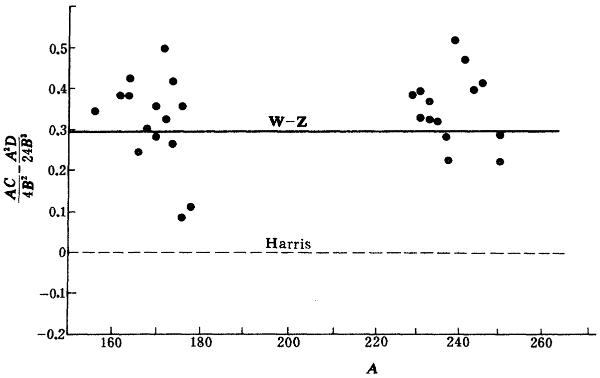

FIG. 3. $(AC/4B^2 - A^2D/24B^3)$ vs A plot.

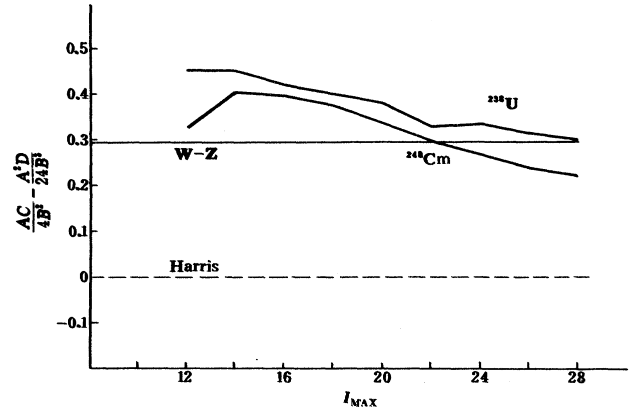

FIG. 4. $(AC/4B^2 - A^2D/24B^3)$ vs $I_{\max}$ plots for ^{238}U and ^{249}Cm.

pressions, the convergence of $I(I+1)$ expansion is not so bad. However, the values of the $I(I+1)$ expansion coefficients obtained by the least-squares fitting deviate significantly from the relations (5) predicted by the two-parameter Harris formula (4), but are close to the relations (8) derived from the two-parameter closed expression (7) for rotational spectra (see Tables I and II and Figs. 1 and 2). Of course, it should be noted that the expression (7) is equivalent to an infinite series of $I(I+1)$ when $I < I_r$ (the radius of convergence, $\approx 1/\sqrt{b}$).[6] Therefore the coefficients deduced from the finite $I(I+1)$ may not coincide exactly with the relation (8).

In addition, according to the relations (5), we have

$$\frac{AC}{4B^2} - \frac{A^2D}{24B^3} = 0 , \tag{10}$$

but, from the relations (8), we get

$$\frac{AC}{4B^2} - \frac{A^2D}{24B^3} = \frac{7}{24} . \tag{11}$$

The $(AC/4B^2 - A^2D/24B^3)$ vs A plot is shown in Fig. 3. We can see that the observed results definitely deviate from the Harris relation (10), but are close to the relation (11).

Finally, the values of coefficients A, B, C, and D, hence $(AC/4B^2 - A^2D/24B^3)$, depend on the number of energy levels involved in the least-squares fitting. For each of the sets of $I = 0, 2, 4, \ldots, I_{\max}$ ($10 \le I_{\max} \le$ the observed highest member below bandcrossing in the GRB), we can obtain a set of values of A, B, C, and D. As two typical examples, the $(AC/4B^2 - A^2D/24B^3)$ vs $I_{\max}$ plots for ^{238}U and ^{248}Cm are shown in Fig. 4. Also we can see that the observed results are close to the relation (11), but do not agree with the relation (10).

[1] A. Bohr and B. R. Mottelson, *Nuclear Structure,* Vol. II, *Nuclear Deformations* (Benjamin, New York, 1975).
[2] S. M. Harris, Phys. Rev. Lett. **13**, 663 (1964); Phys. Rev. **138B**, 509 (1965).
[3] For example, see R. Bengtsson and J. D. Garrett, Int. Rev. Nucl. Phys. **2**, 193 (1984).
[4] Ø. Seathre, S. A. Hjorth, A. Johnson, S. Jagare, H. Ryde, and Z. Szymanski, Nucl. Phys. **A207**, 486 (1973).
[5] B. R. Mottelson, Proceedings of the Nuclear Structure Symposium of the Thousand Lakes, Joutsa, 1970 [Nordisk Institut for Theoretisk Atomfysik, Nordita, Report No. 417 (unpublished)].
[6] C. S. Wu and J. Y. Zeng, Commun. Theor. Phys. (Beijing) **8**, 51 (1987).
[7] H. X. Huang, C. S. Wu, and J. Y. Zeng, Phys. Rev. C **39**, 1617 (1989).
[8] J. Y. Zeng, C. S. Wu, H. W. Huang, and J. L. Wood (submitted to Nucl. Phys. A).
[9] T. Czosnyka, D. Cline, L. Hasselgren, C. Y. Wu, R. M. Diamond, H. Kluge, C. Roulet, E. K. Hulet, R. W. Lougheed, and C. Baktash, Nucl. Phys. **A458**, 123 (1986).
[10] P. B. Piercey, J. H. Hamilton, A. V. Ramayya, H. Emling, P. Fuchs, E. Grosse, D. Schwalm, H. J. Wollersheim, N. Trautmann, A. Faessler, and M. Ploszajczak, Phys. Rev. Lett. **46**, 415 (1981).
[11] E. N. Shurshikov, Nucl. Data Sheets **49**, 785 (1986).
[12] E. N. Shurshikov, Nucl. Data Sheets **45**, 509 (1985).
[13] K. Hardt, P. Schüler, C. Günther, J. Recht, and K. P. Blume, Nucl. Phys. **A407**, 127 (1983).
[14] M. Sakai, At. Data Nucl. Data Tables **31**, 399 (1984).
[15] H. Ower, Th. W. Elze, J. Idzko, K. Stelzer, E. Grosse, H. Emling, P. Fuchs, D. Schwalm, H. J. Wollersheim, N. Kaffrell, and N. Trautmann, Nucl. Phys. **A388**, 421 (1982).
[16] Y. A. Ellis-Akovali, Nucl. Data Sheets **40**, 523 (1983).
[17] A. M. Y. El-Lawindy, L. D. Burrows, P. A. Butler, A. N. James, G. D. Jones, T. P. Morrison, J. Simpson, K. A. Connell, R. Wadsworth, and D. L. Watson, J. Phys. G **12**, 1059 (1986).
[18] M. J. Martin, Nucl. Data Sheets **49**, 83 (1986).
[19] D. J. Horen and B. Harmatz, Nucl. Data Sheets **19**, 383 (1986).
[20] E. Browne, Nucl. Data Sheets **41**, 277 (1983).
[21] Wang Gong Qing, Nucl. Data Sheets **45**, 509 (1985).
[22] Zhou Chunmei, Nucl. Data Sheets **50**, 351 (1987).
[23] A. E. Ignatochkin, E. N. Shurshikov, and Yu. F. Jaborov, Nucl. Data Sheets **52**, 365 (1987).
[24] E. N. Shurshikov, Nucl. Data Sheets **47**, 433 (1986).
[25] R. G. Helmer, Nucl. Data Sheets **44**, 659 (1985).
[26] R. G. Helmer, Nucl. Data Sheets **49**, 383 (1986).