Octupole deformations from DFT

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The Workshop on the Nuclear Octupole Degree of Freedom
July 25th & 26th 2019
University of the West of Scotland in Paisley, UK

University of York

Science & Technology Facilities Council

UK Research and Innovation

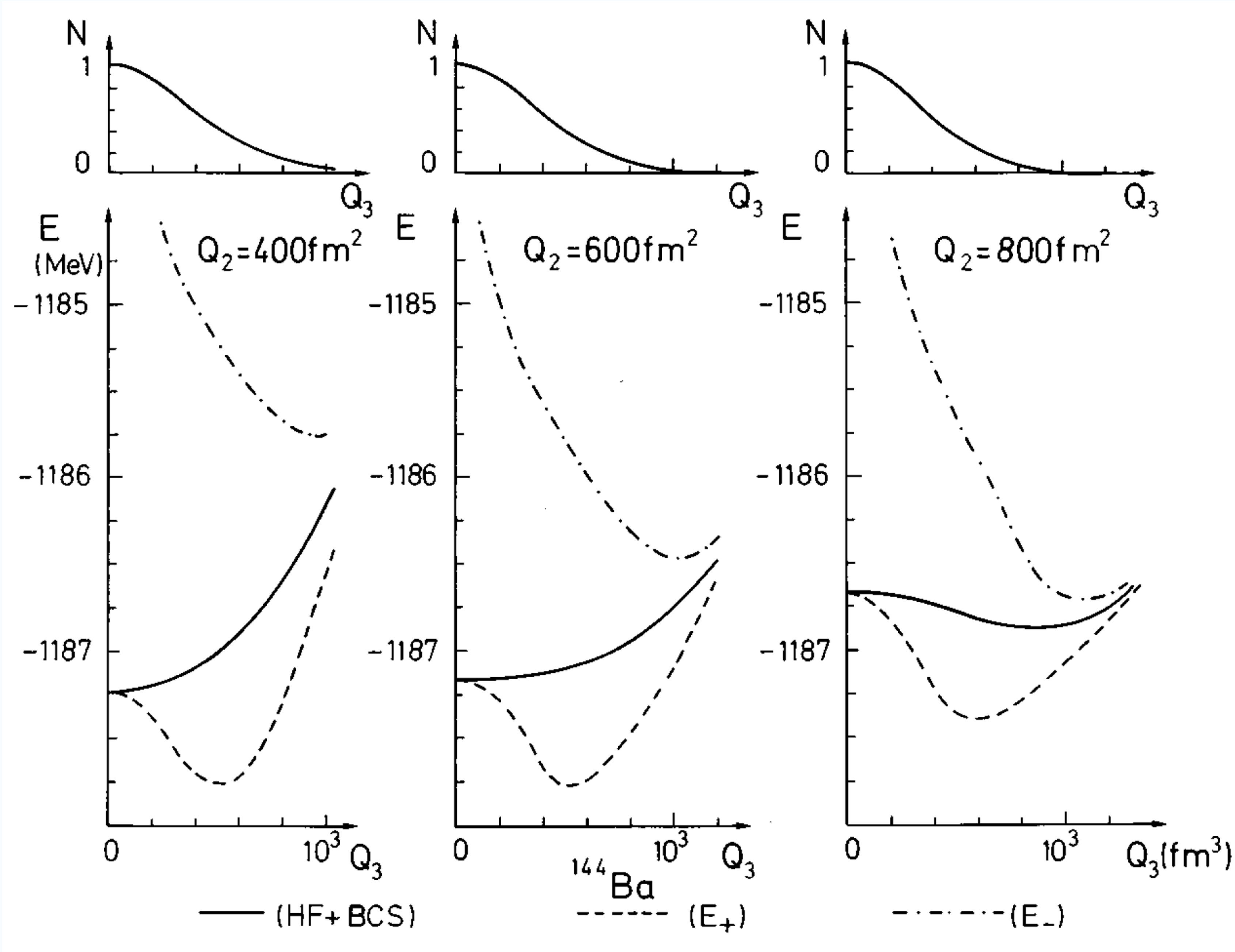
University of Warsaw

Outline

1. Nuclear octupole moments
2. Correlations between the Schiff and octupole moments
3. Configurations, magnetic dipole moments, and electric quadrupole moments in ^{229}Th
4. Octupole collectivity in ^{143}Ba
5. Conclusions and further work

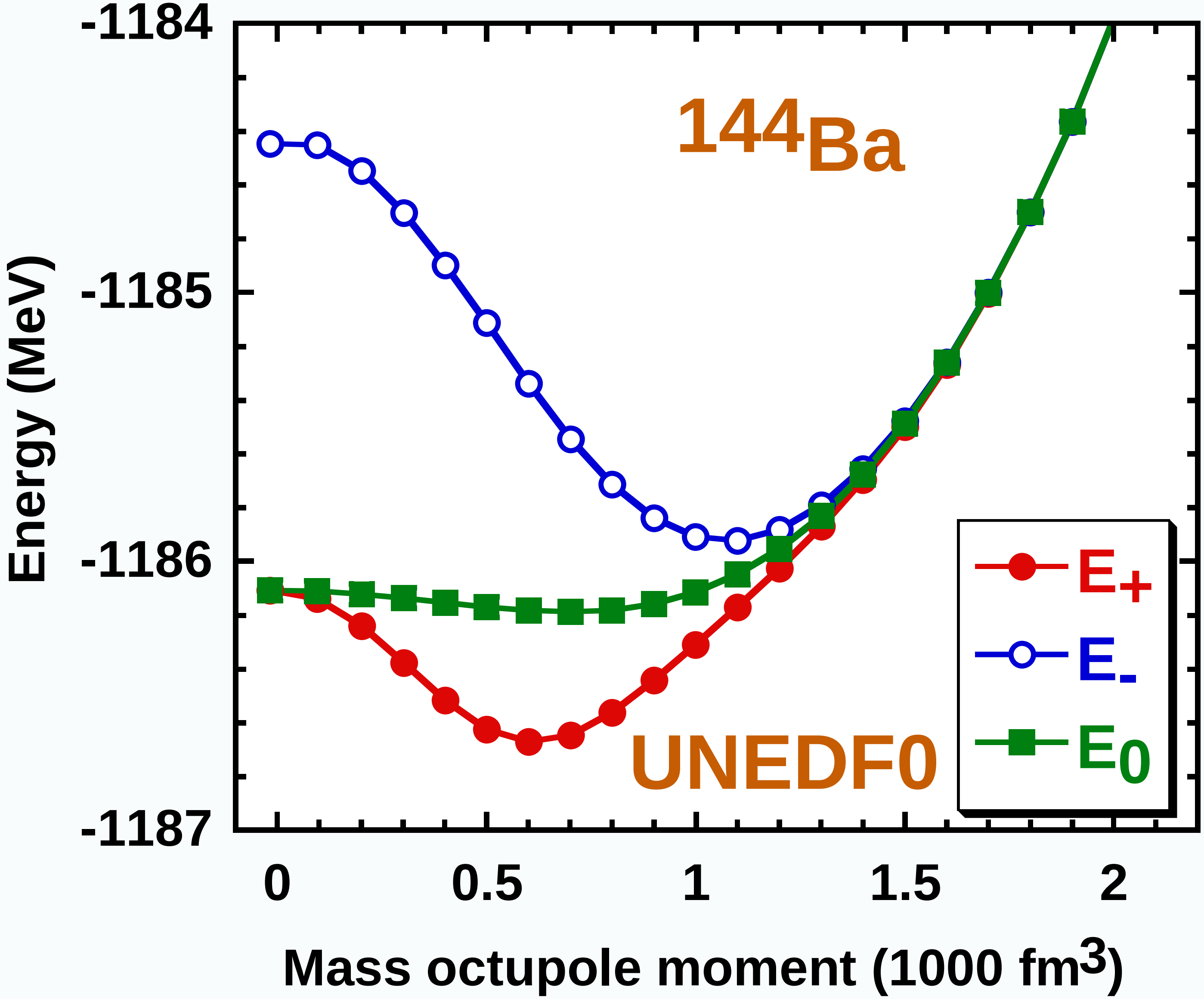
In collaboration with Pierre Becker, Jonathan Engel, Markus Kortelainen, and Alessandro Pastore

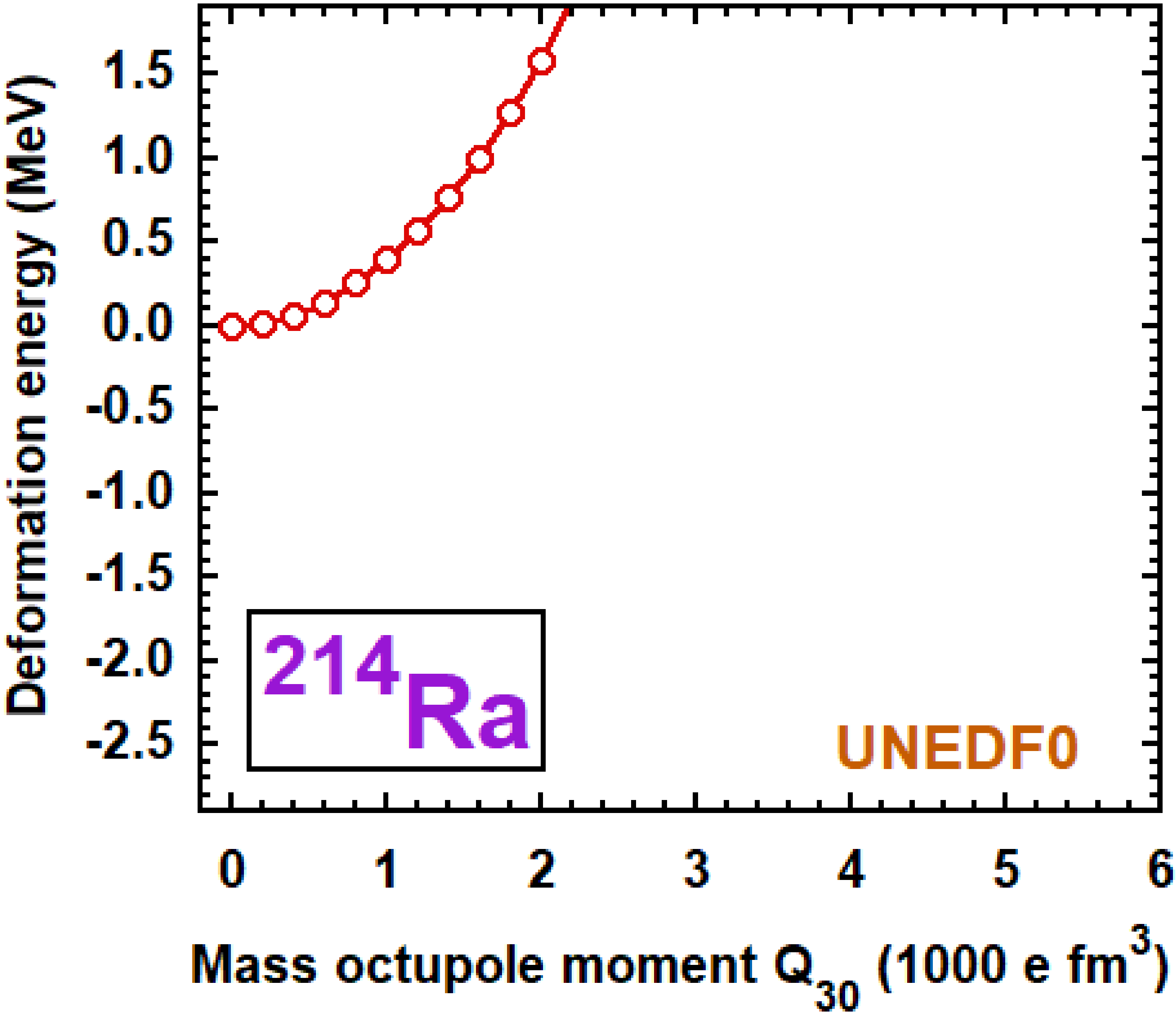
Prelude



Butler and Nazarewicz
Reviews of Modern Physics, Vol. 68, No. 2, April 1996
From Bonche, P., 1988, in The Variety of Nuclear Shapes
edited by J.D. Garrett et al. (World Scientific, Singapore), p. 302.

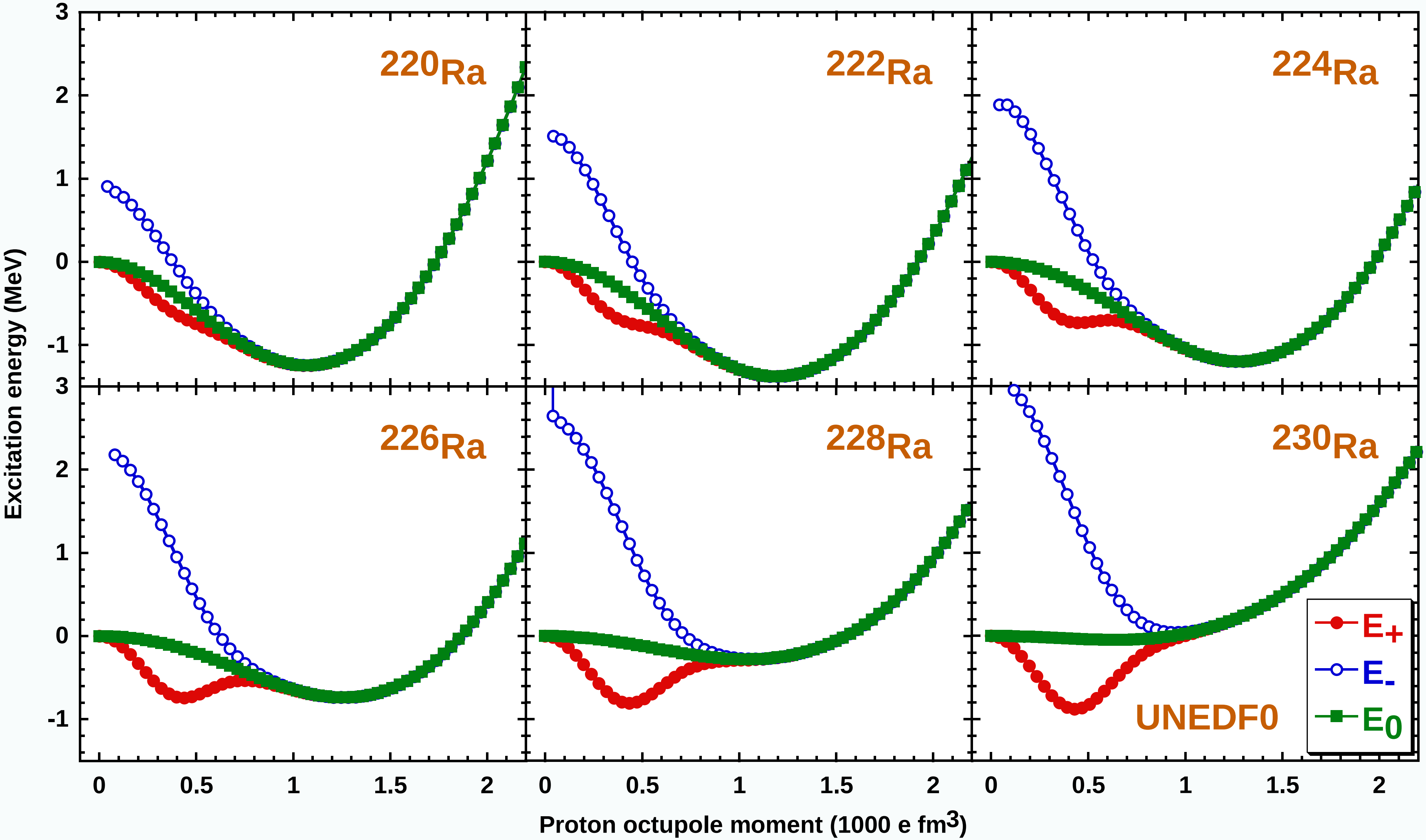
$$E_{\pm}=(E_0\pm\Delta)/(1\pm\varepsilon)$$





Deformation energy (MeV)
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
0
1
2
3
4
5
6
Mass octupole moment Q30 (1000 e fm3)
214Ra
UNEDF0

$E_{\pm}=(E_0\pm\Delta)/(1\pm\varepsilon)$



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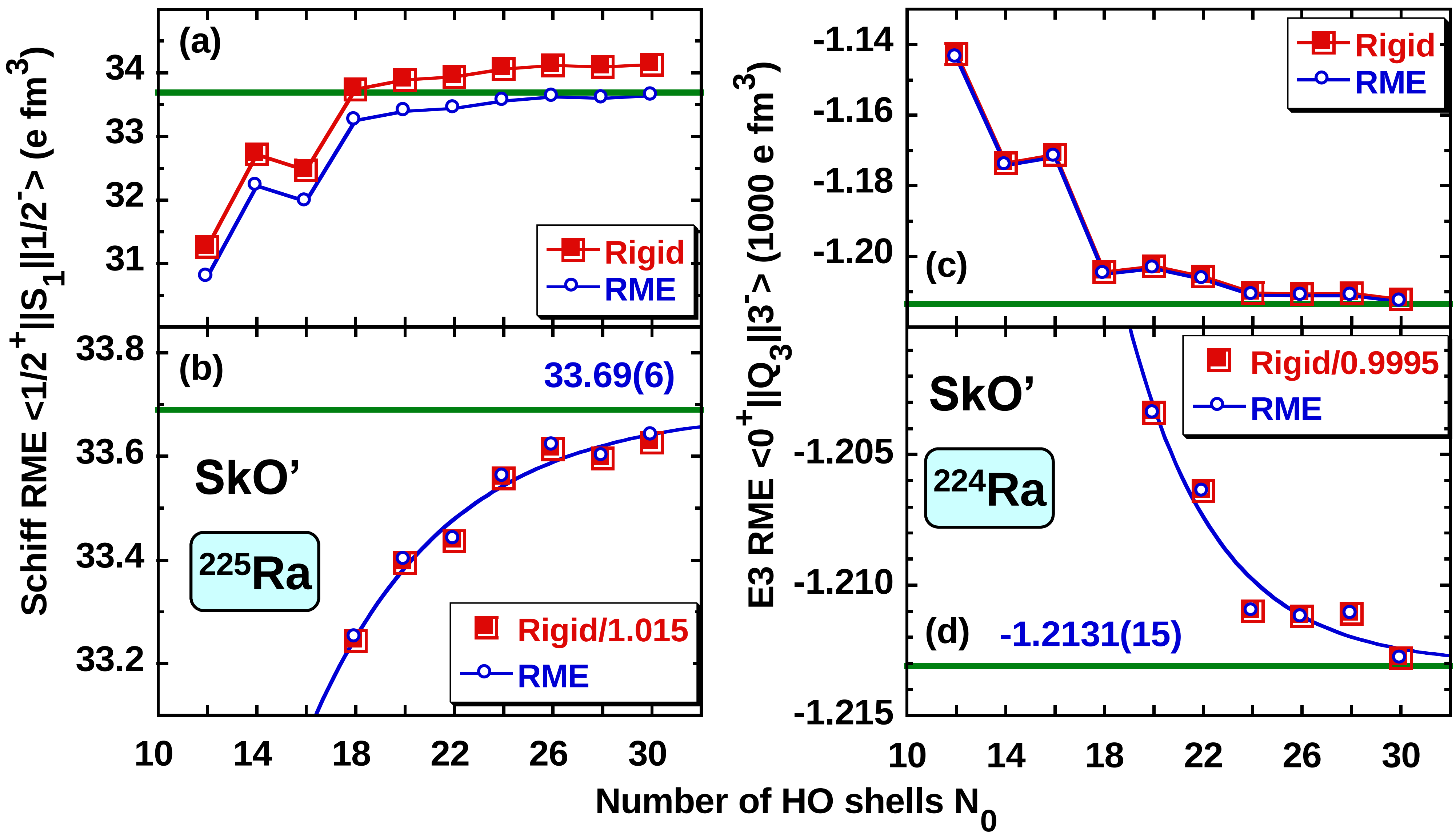
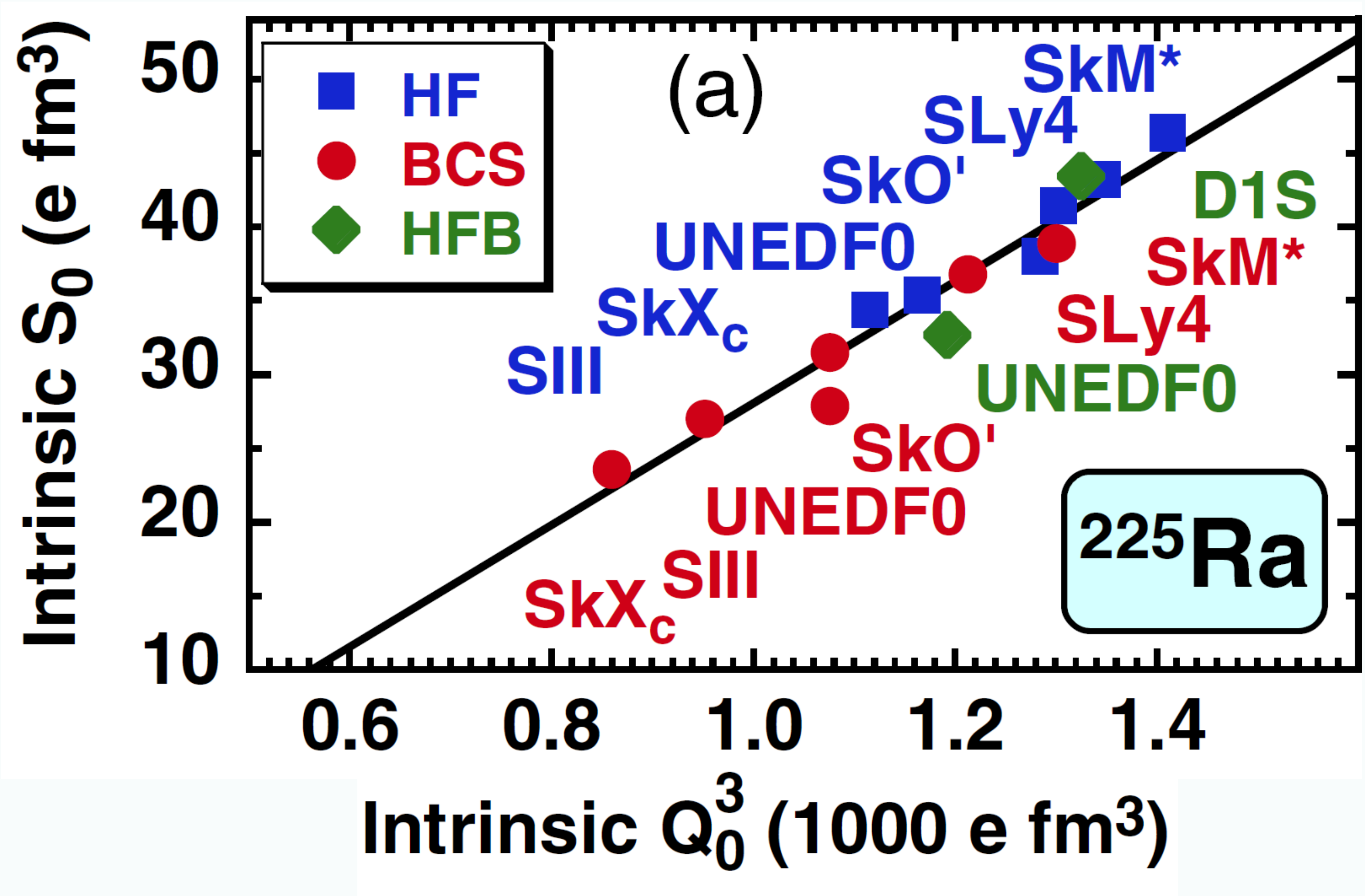
Schiff vs. octupole

Quality of the rotational approximation to the reduced matrix elements is excellent

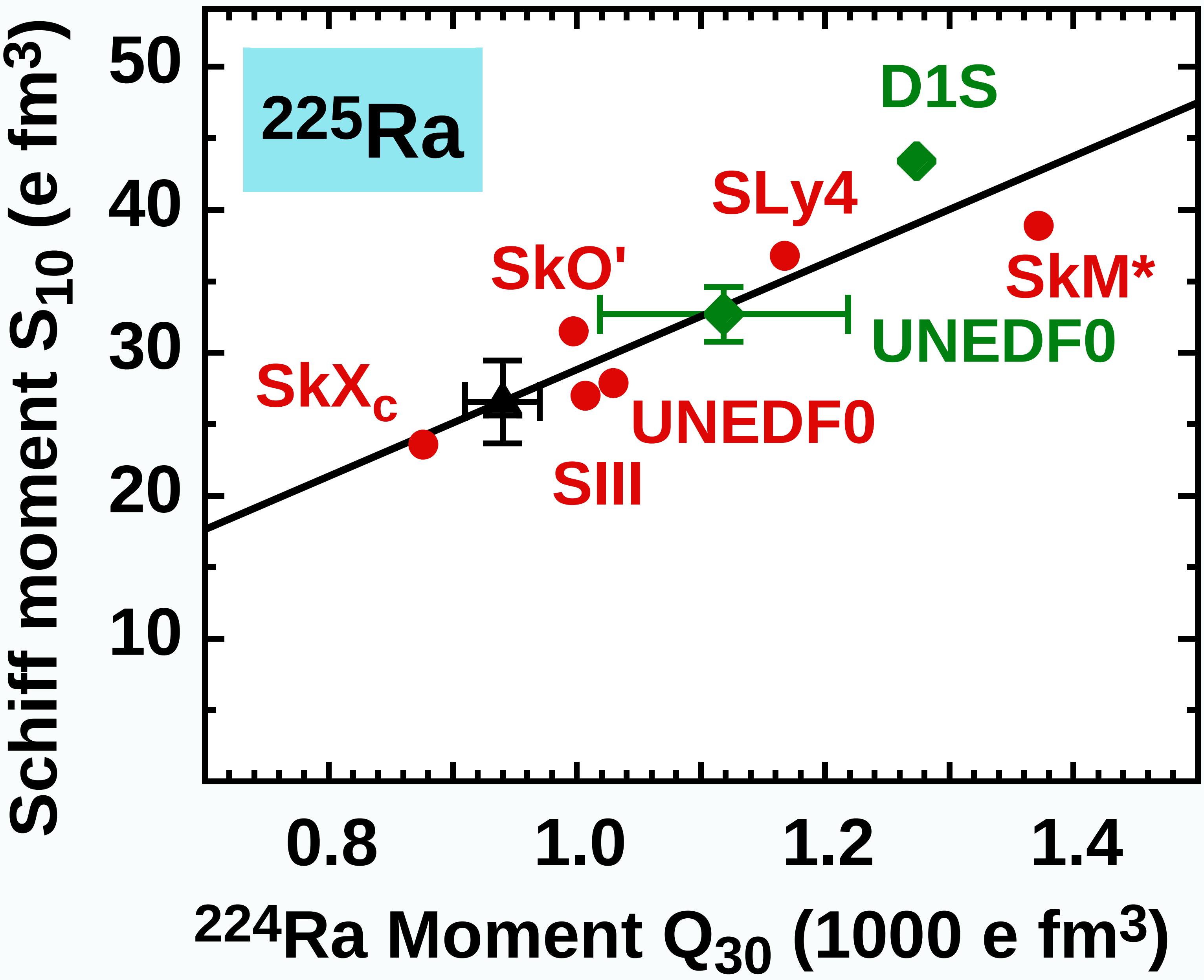


^{225}Ra Schiff moment vs. ^{225}Ra octupole moment

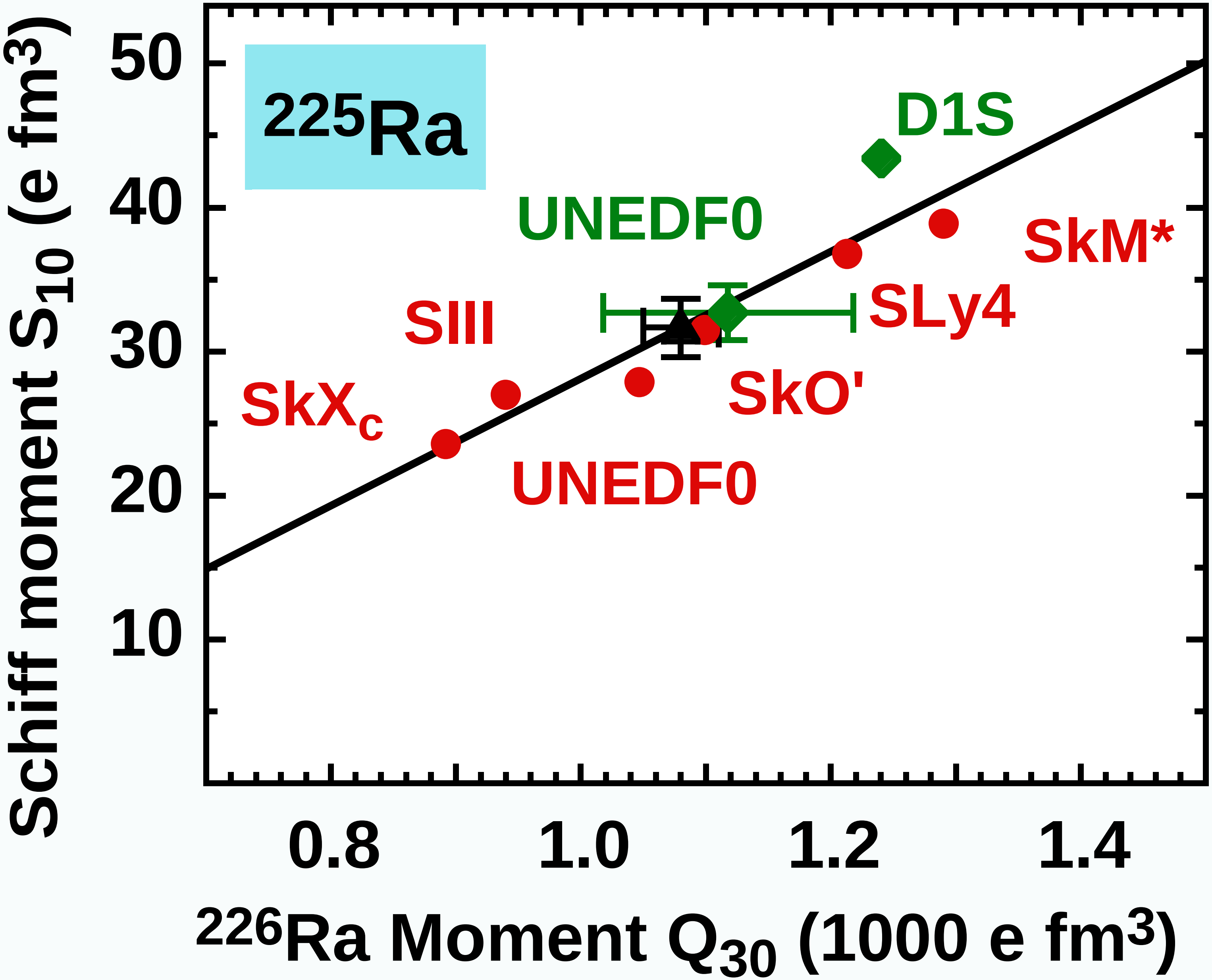


J.D., J. Engel, M. Kortelainen, P. Becker, Phys. Rev. Lett., 121, 232501 (2018)

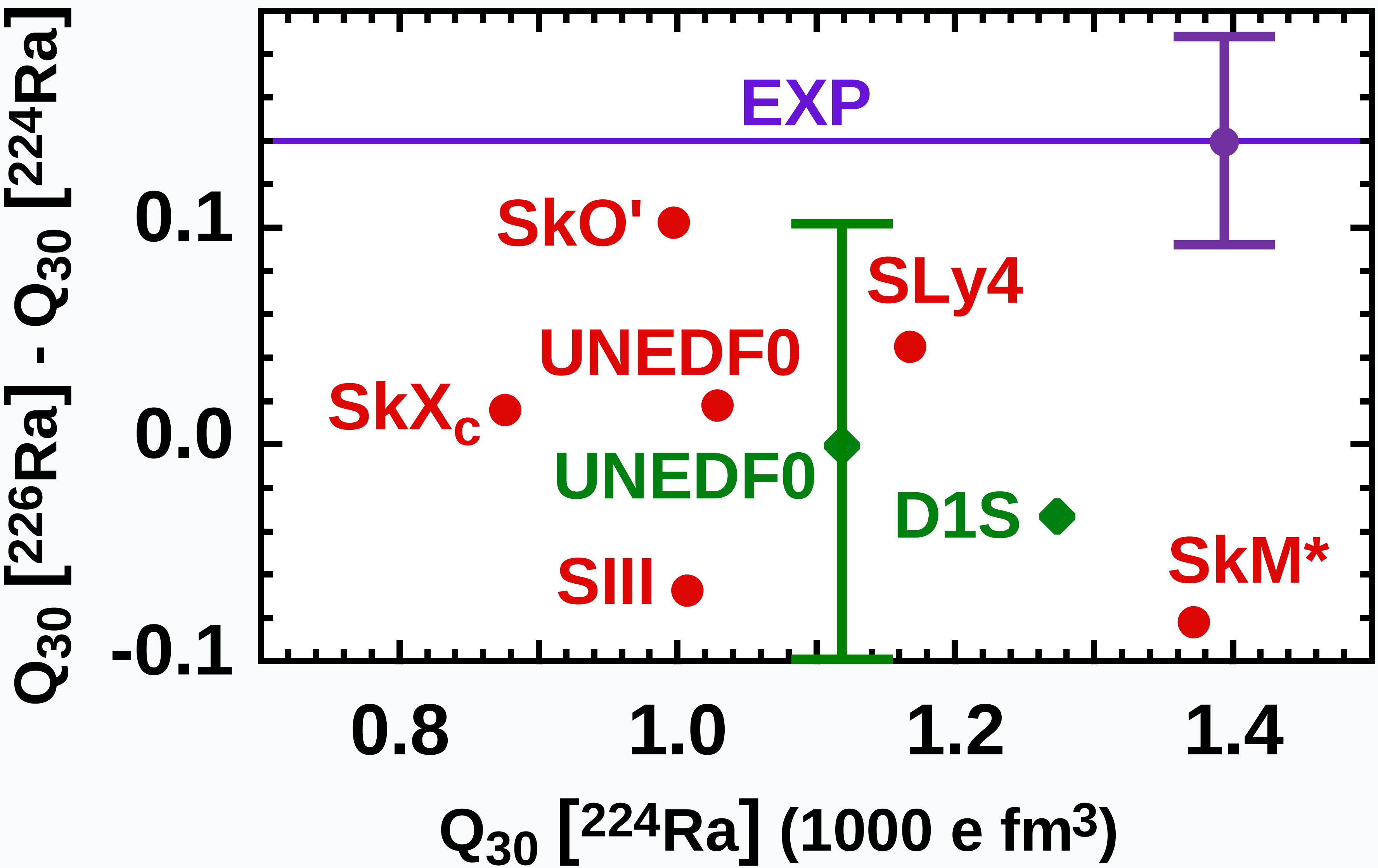
^{225}Ra Schiff moment vs. ^{224}Ra octupole moment



^{225}Ra Schiff moment vs. ^{226}Ra octupole moment

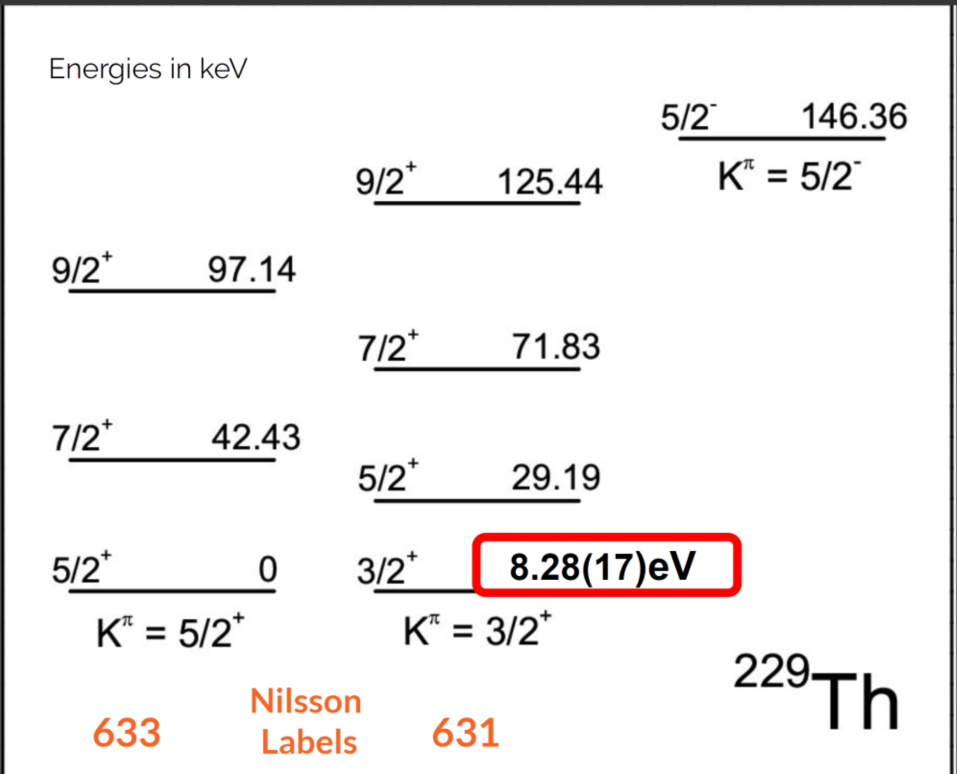


Octupole moments in ^{224}Ra and ^{226}Ra



^{229}Th

What is known about ^{229m}Th?



What we can aim for

1. Binding energies
2. **Odd-Even Mass Staggering**
3. **Axially and octupolly deformed**
4. Half-life
5. **Proton Quadrupole moments**
6. **Magnetic dipole moment**
7. Mean_square radii difference
8. **First few transition rates**

Δ_n = 0.77 MeV

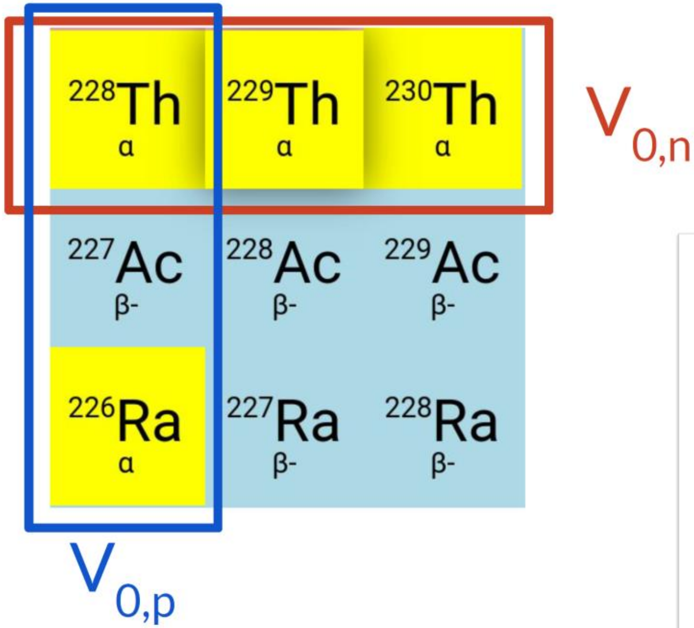
Δ_p = 0.68MeV

Octupole: degree of freedom

$Q_{5/2}$= 8.8(1) eb
$Q_{3/2}$= 8.7(3) eb

$\mu_{5/2}$= 0.360(7) μ_N
$\mu_{3/2}$= -0.37(6) μ_N

Reproduction of experimental odd-even mass staggering



Source:
https://people.physics.anu.edu.au/~ecs103/chart/

Experimental values to reproduce:

Δ_n = 0.77 MeV

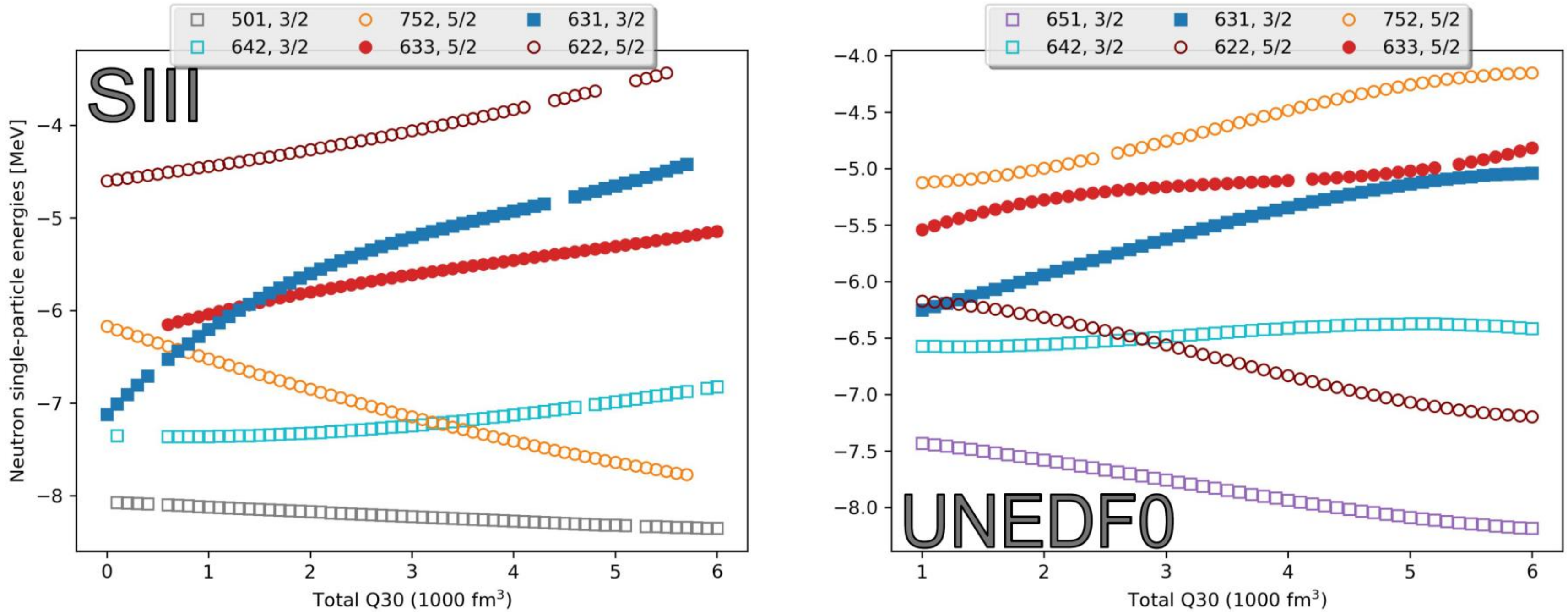
Δ_p = 0.68MeV

Adjusted pairing

Interaction	$V_{0,n}$	$V_{0,p}$
SIII	181.15	220.19
SKM*	181.46	216.25
SKO'	163.82	184.34
SKXc	139.02	173.63
SLY4	207.76	231.89
UDF0	130.70	156.45
UDF1	145.35	169.80

Let's go crossing hunting

SIII used before for 229Th calculations:
E.Litvinova *et al.*,Phys. Rev.C, 79 064303 (2009)



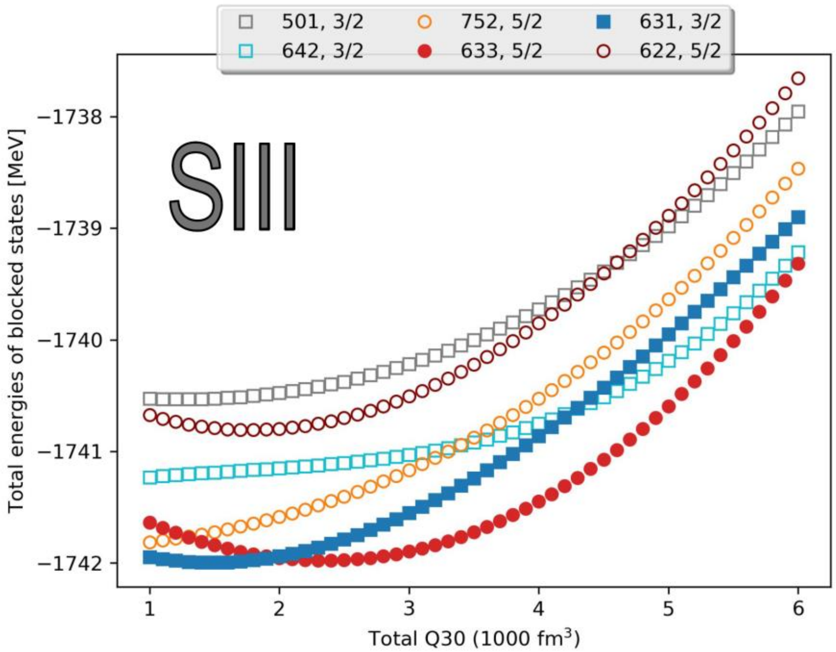
Evolution of the energy of the blocked state with the octupole deformation in ^{229}Th

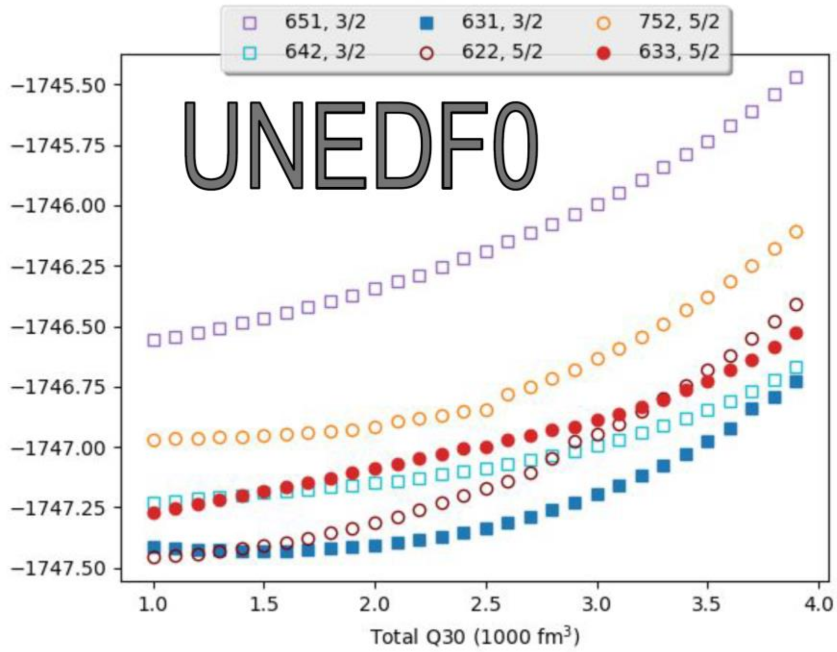
Exploring Skyrme parame-trisations

Results obtained while fitting pairing strengths

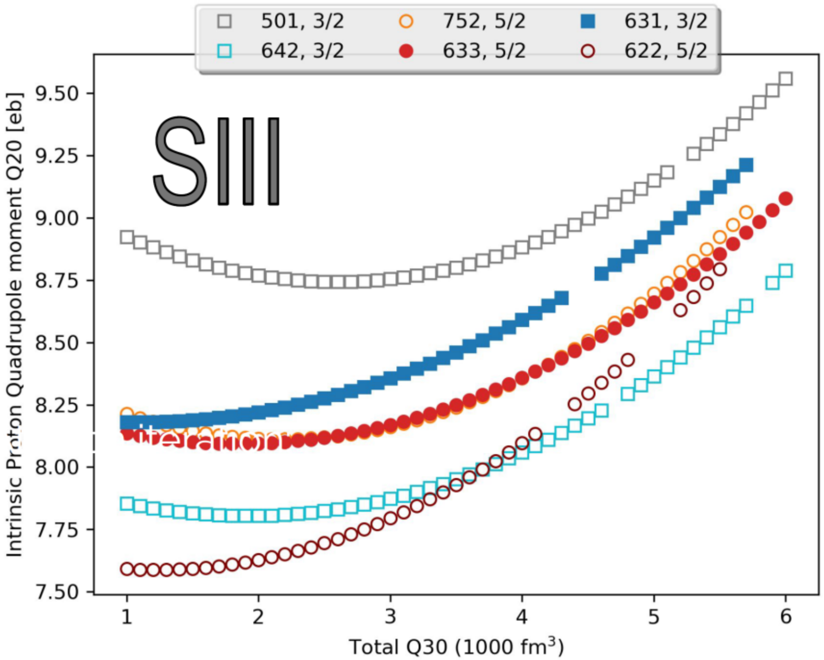
^{229}Th **is not in the fitting constrains** for these interactions, so **no systematics** expected.

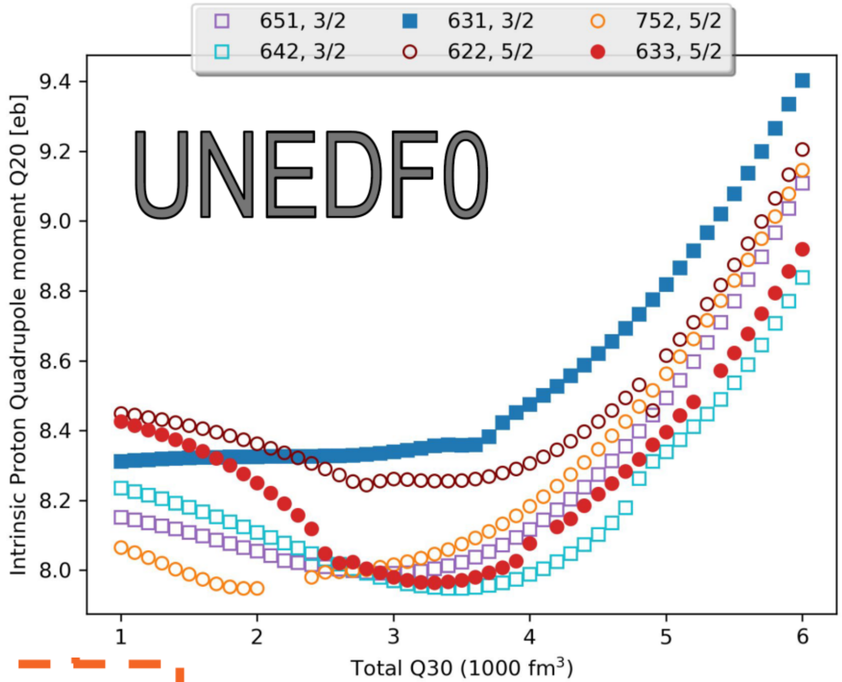
Parametrisations	Proton Q_{20} (100 fm)	Proton Q_{30} (1000 fm)	Magnetic moment (μ_N)
SIII | 631, 3/2> | 633, 5/2>	8.17 8.13	1.70 2.25	-0.52 0.16
SKM* | 631, 3/2> | 752, 5/2>	**8.66** 8.65	1.85 0.28	-0.24 -0.53
SKO' | 631, 3/2> | 633, 5/2>	8.41 8.15	1.49 2.89	-0.56 -0.20
SKXc | 631, 3/2> | 633, 5/2>	8.06 8.16	1.31 0.75	-0.53 -0.28
SLY4 | 631, 3/2> | 633, 5/2>	8.51 8.54	2.13 0.68	-0.53 -0.14
UDF0 | 622, 5/2> | 63, 3/2>	8.46 8.32	0.68 1.39	-0.44 -0.44
UDF1 | 752, 5/2> | 631, 3/2>	8.58 8.48	0.66 1.75	-0.40 -0.49





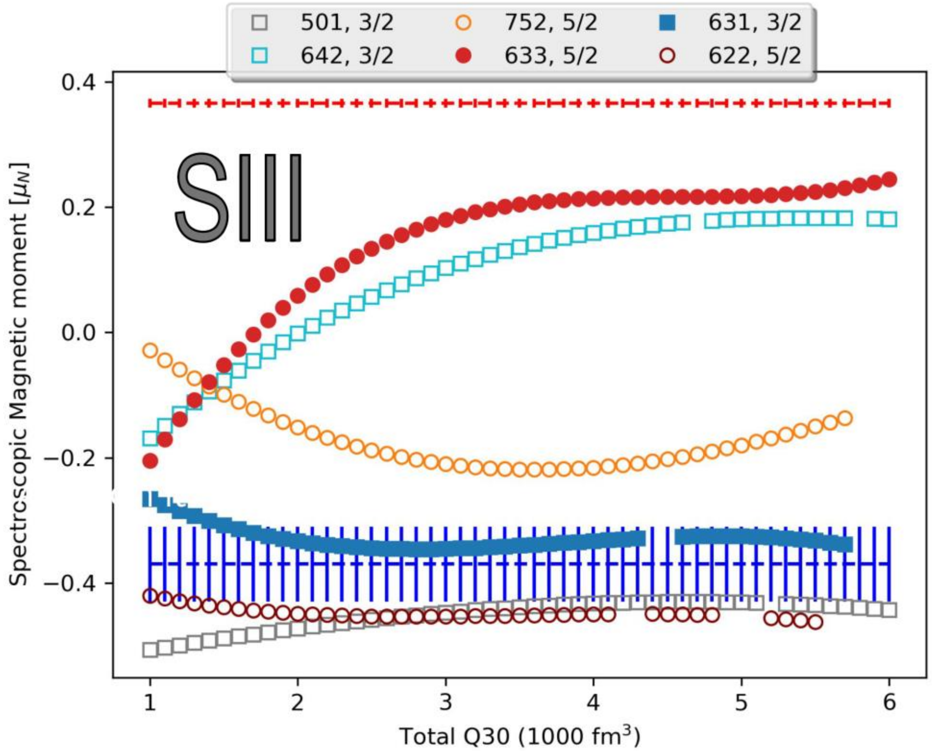
Evolution of the energy for the blocked ^{229}Th total energy

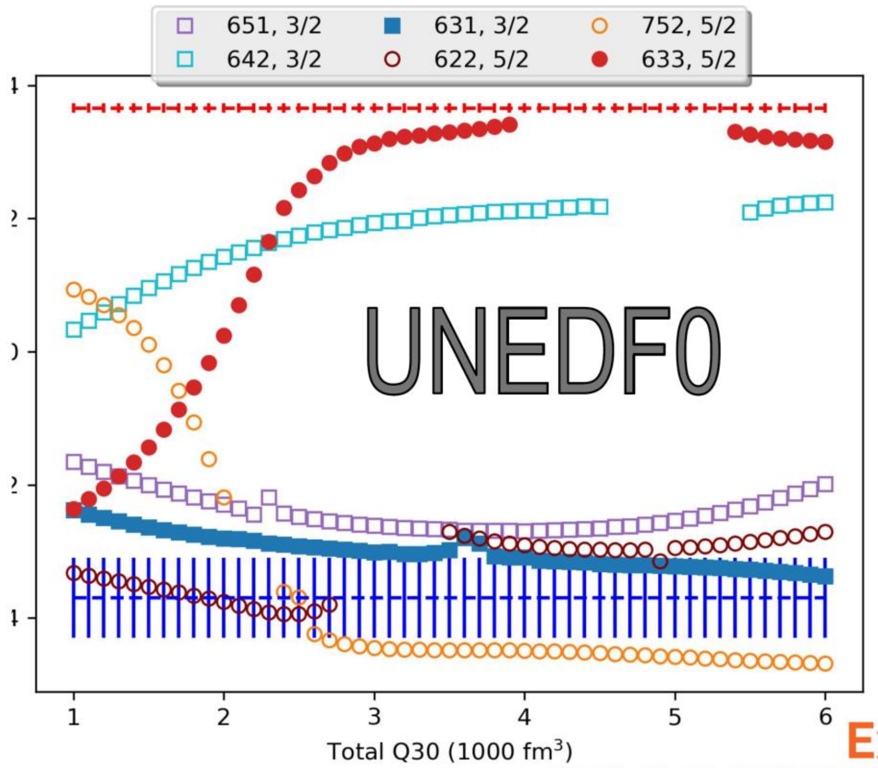




-- $Q_{5/2}$ = 8.8(1) eb
-- $Q_{3/2}$ = 8.7(3) eb

Evolution of the intrinsic proton quadrupole moment for the blocked ^{229}Th





No time-odd terms

Exp

-- $\mu_{5/2}$ = 0.360(7) μ_N
-- $\mu_{3/2}$ = -0.37(6) μ_N

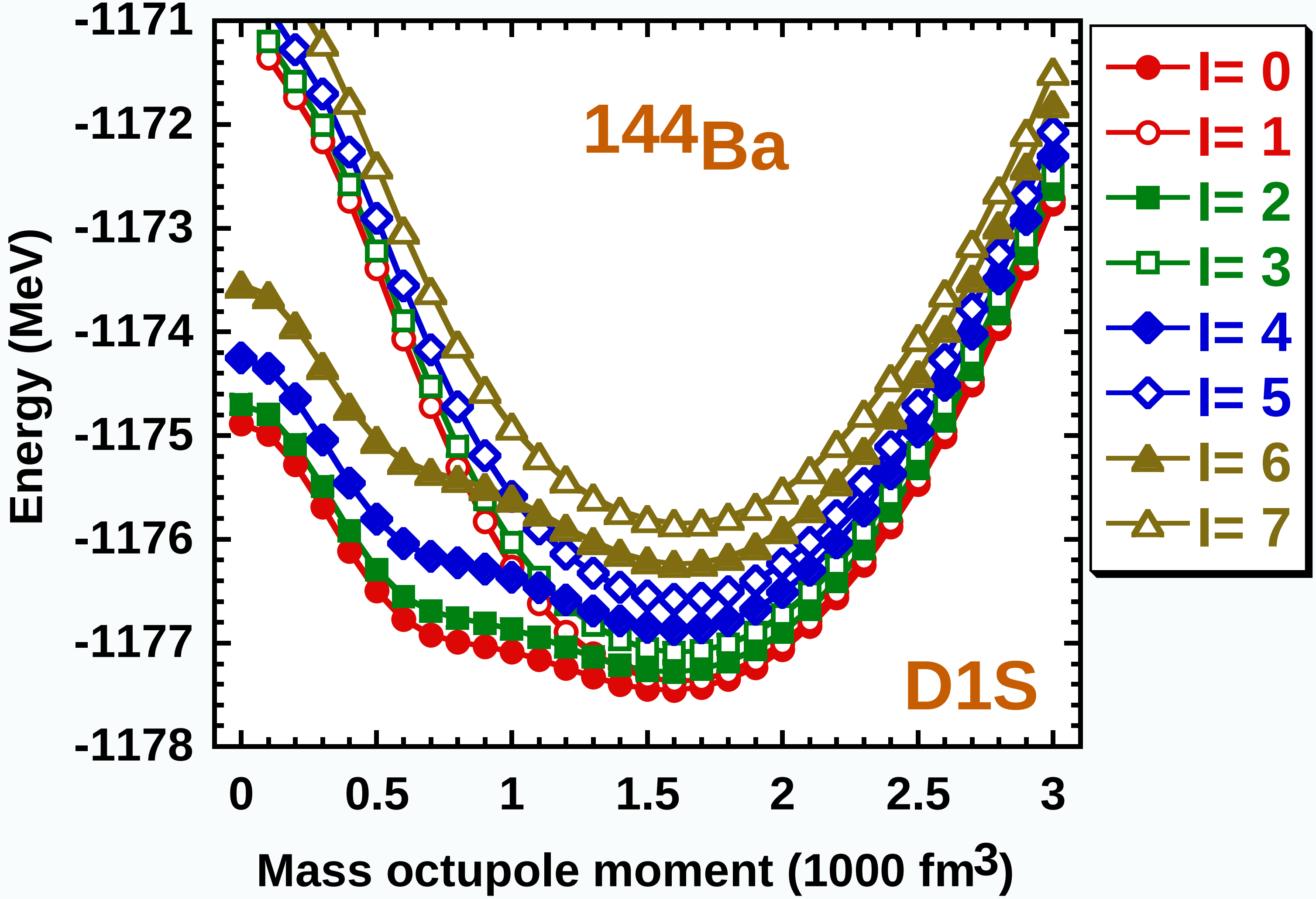
Evolution of the spectroscopic total magnetic moment for the blocked ^{229}Th

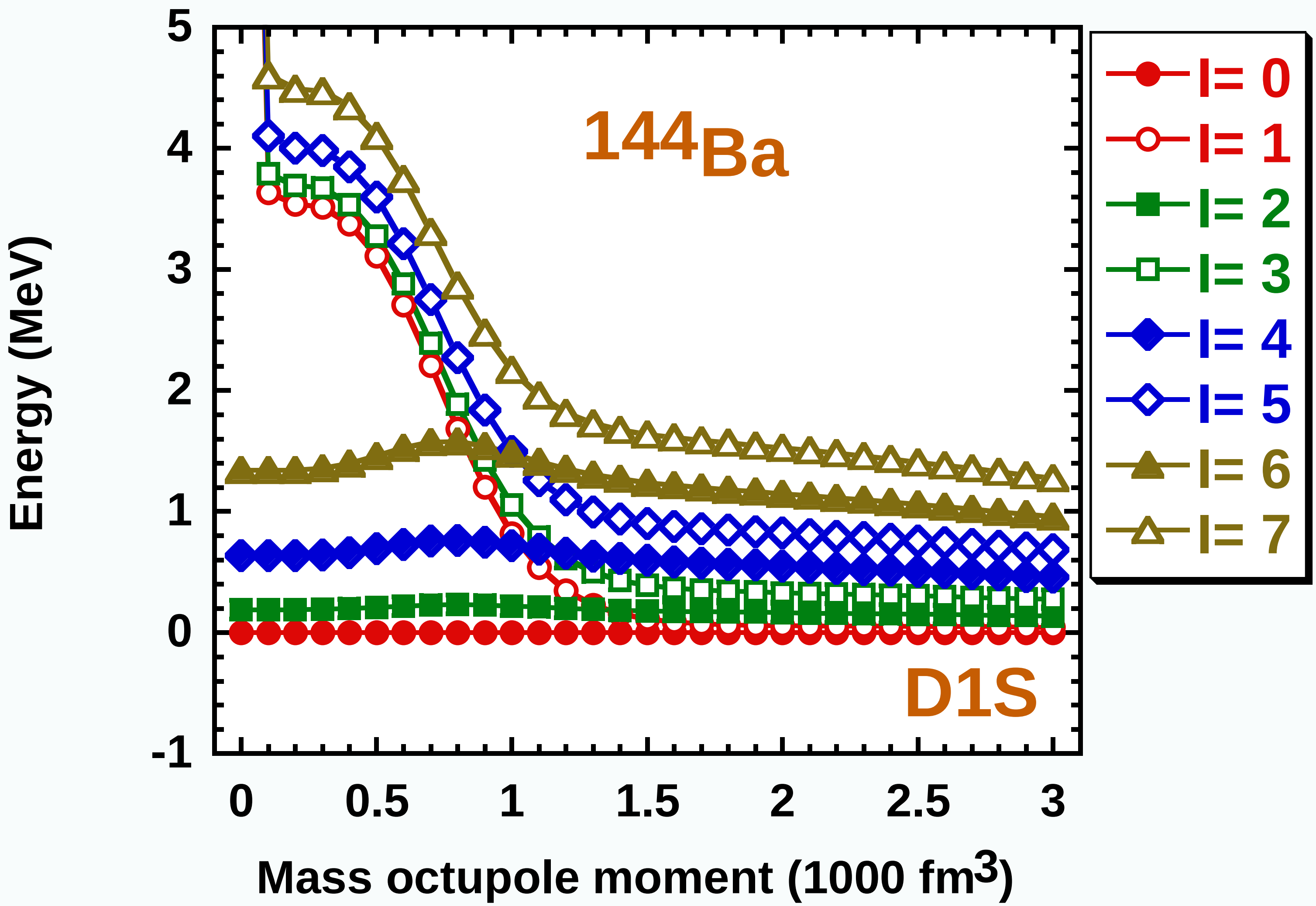
What's next for ^{229}Th?

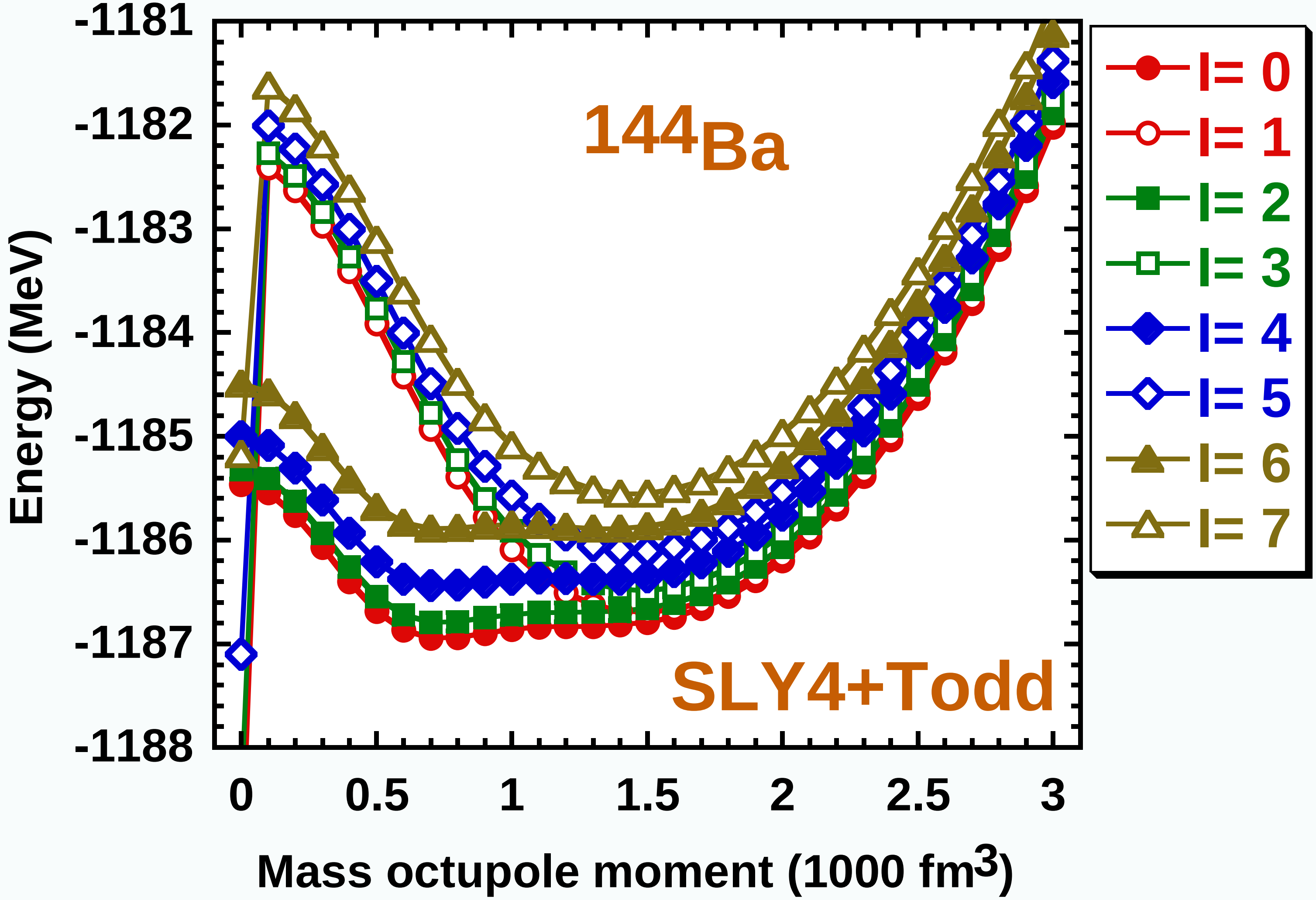
1. Constrain the quadrupole moments to experimental values.
2. Adjust the time-odd coupling constants (Landau parameters) to experimental magnetic moments.
3. Perform the GCM mixing of octupole shapes.
4. Project the particle numbers.
5. Determine the 3/2+ → 5/2+ E2 and M1 reduced matrix elements and their mixing together with their uncertainties.

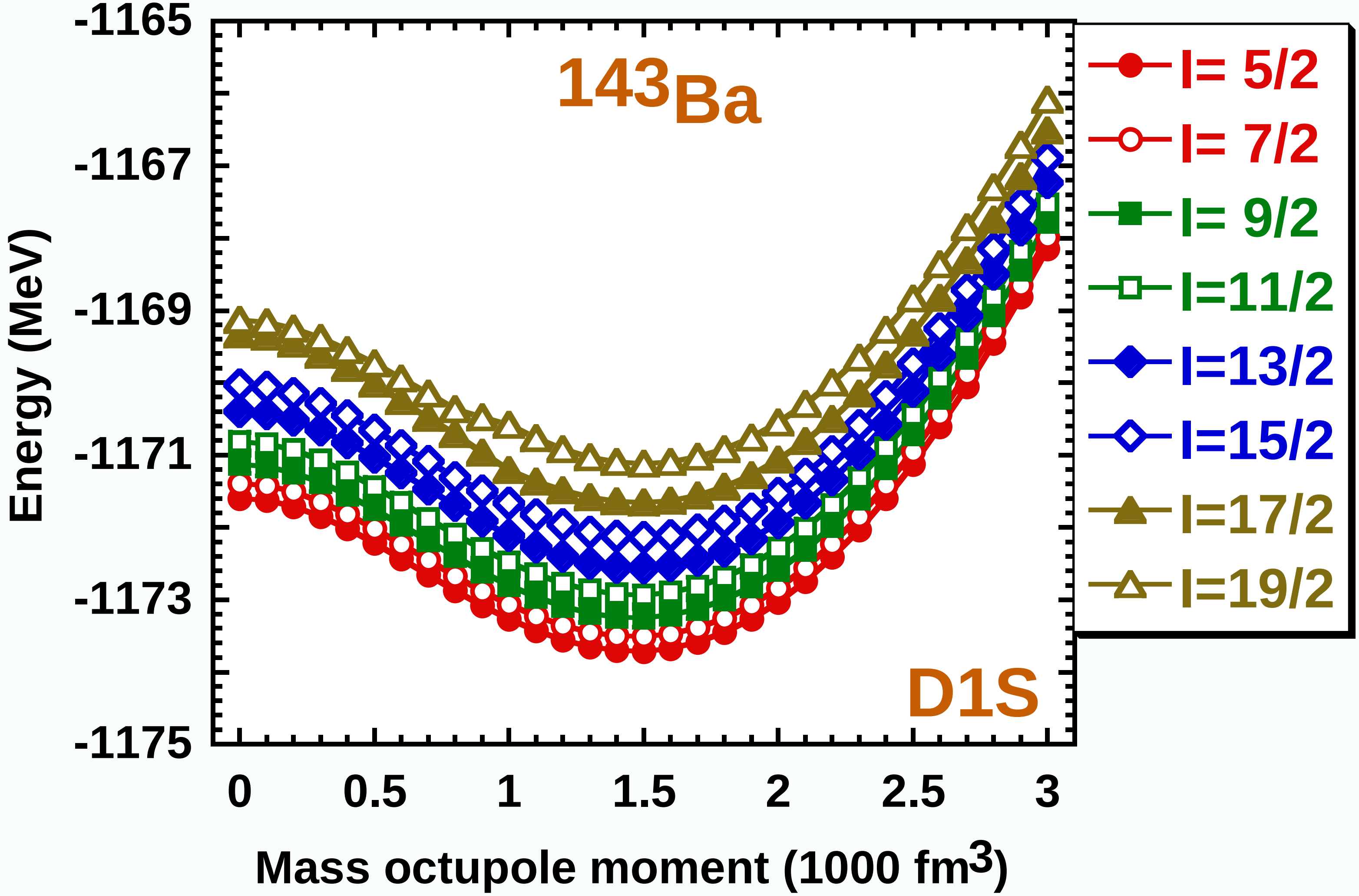
^{144}Ba & ^{143}Ba

(no pairing here and below)

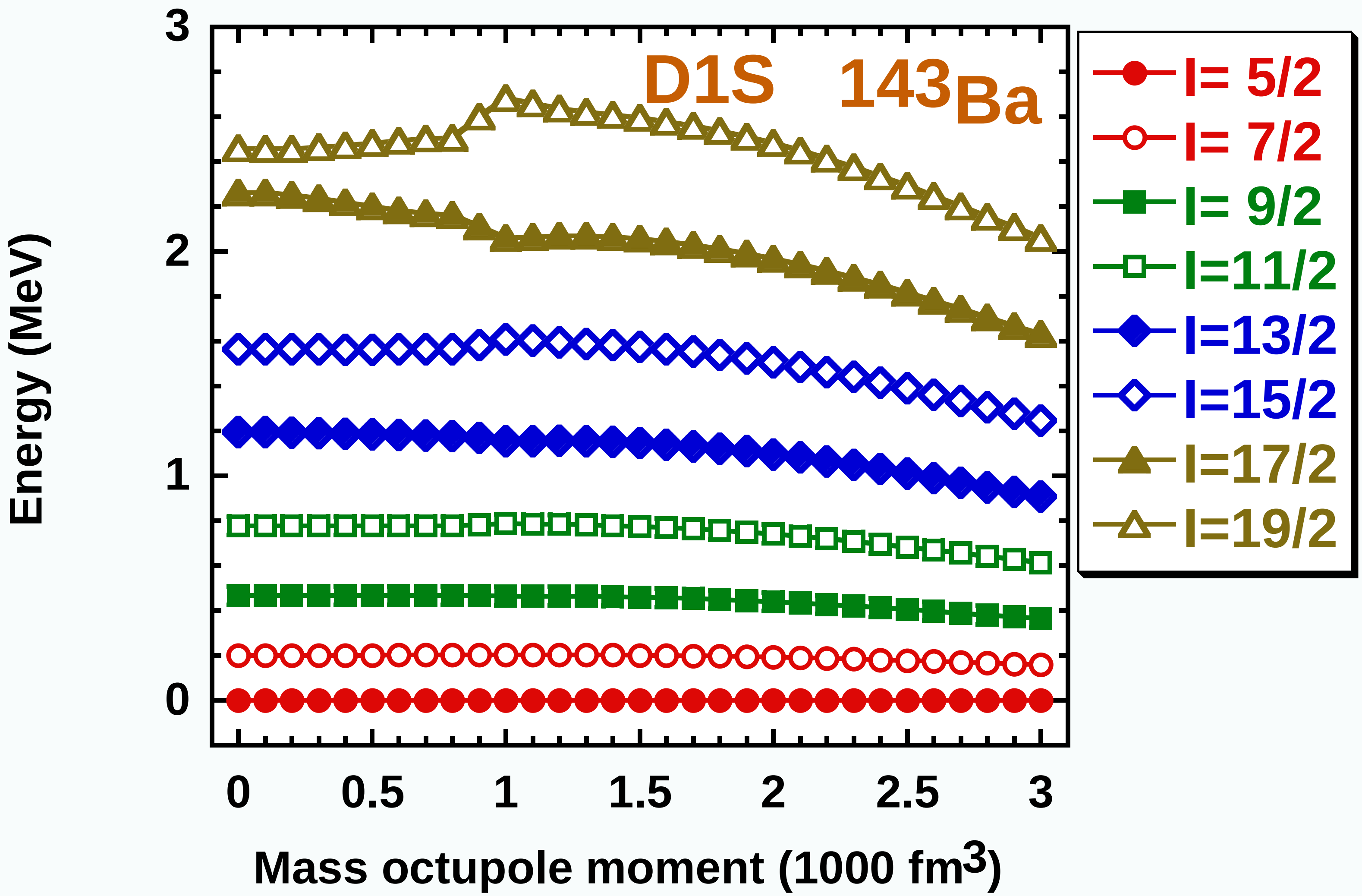


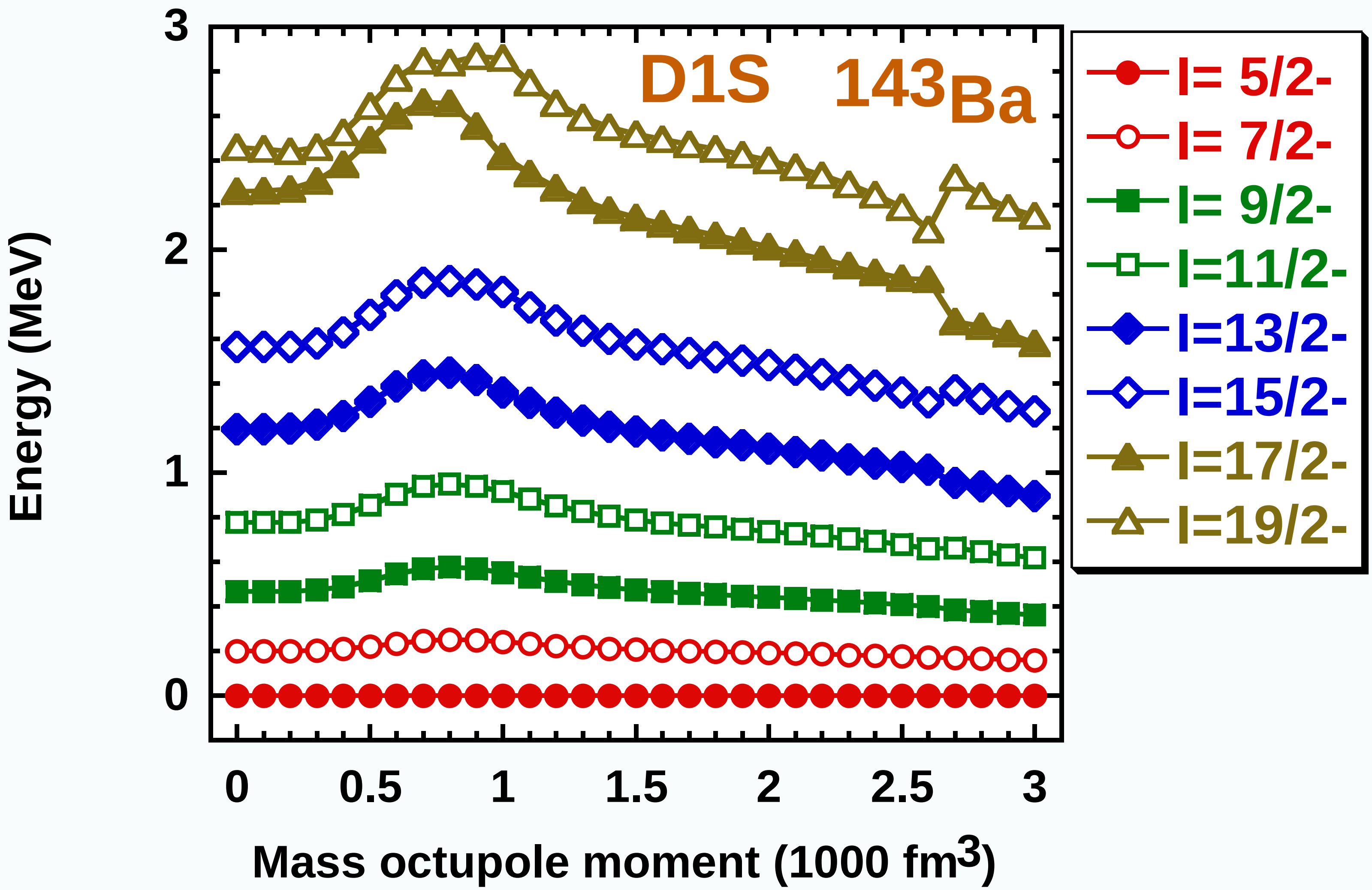

144Ba
D1S
I= 0
I= 1
I= 2
I= 3
I= 4
I= 5
I= 6
I= 7
Energy (MeV)
Mass octupole moment (1000 fm3)
5
4
3
2
1
0
-1
0
0.5
1
1.5
2
2.5
3

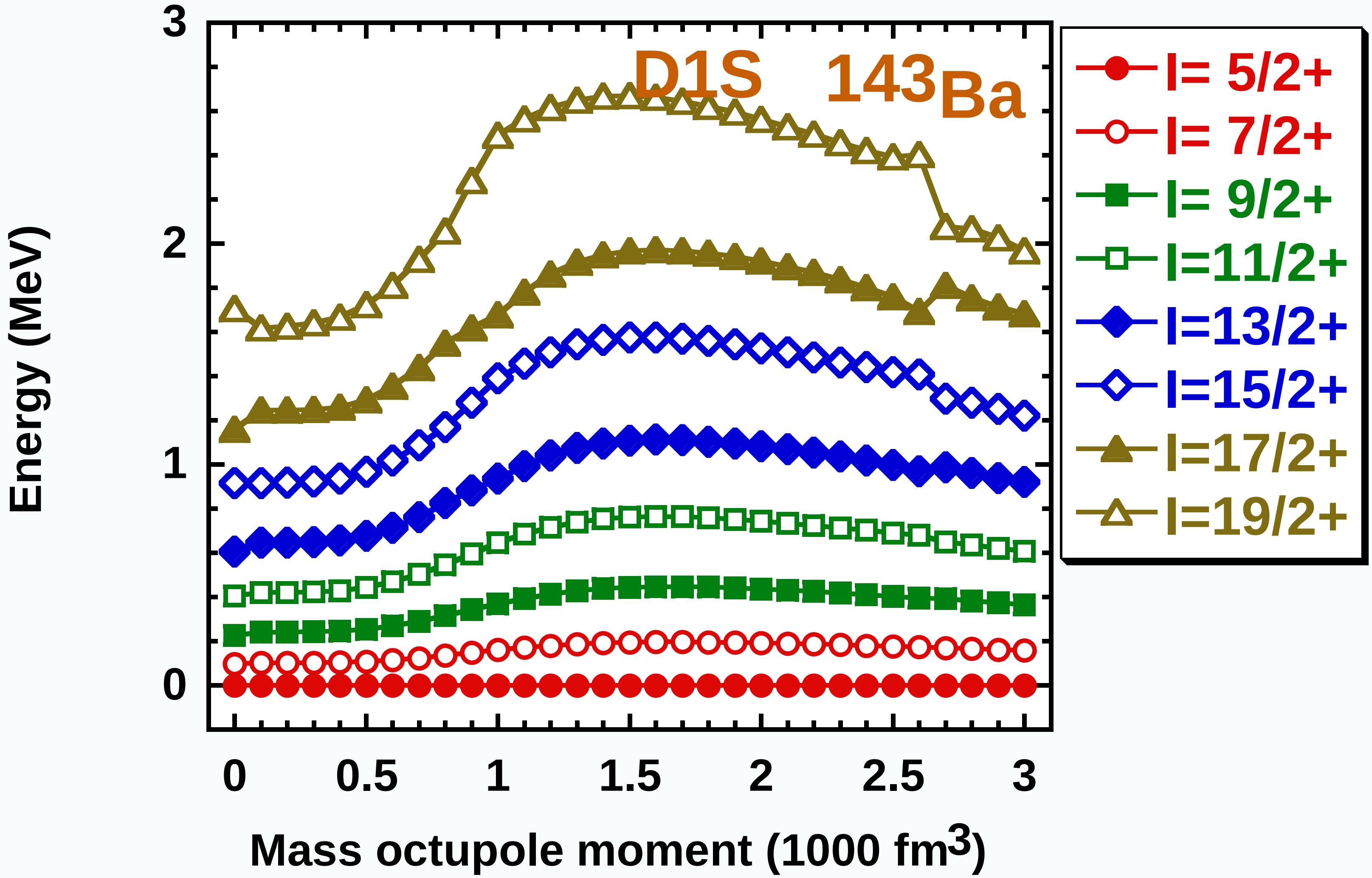

144Ba
SLY4+Todd
Energy (MeV)
Mass octupole moment (1000 fm3)
-1181
-1182
-1183
-1184
-1185
-1186
-1187
-1188
0
0.5
1
1.5
2
2.5
3
I= 0
I= 1
I= 2
I= 3
I= 4
I= 5
I= 6
I= 7



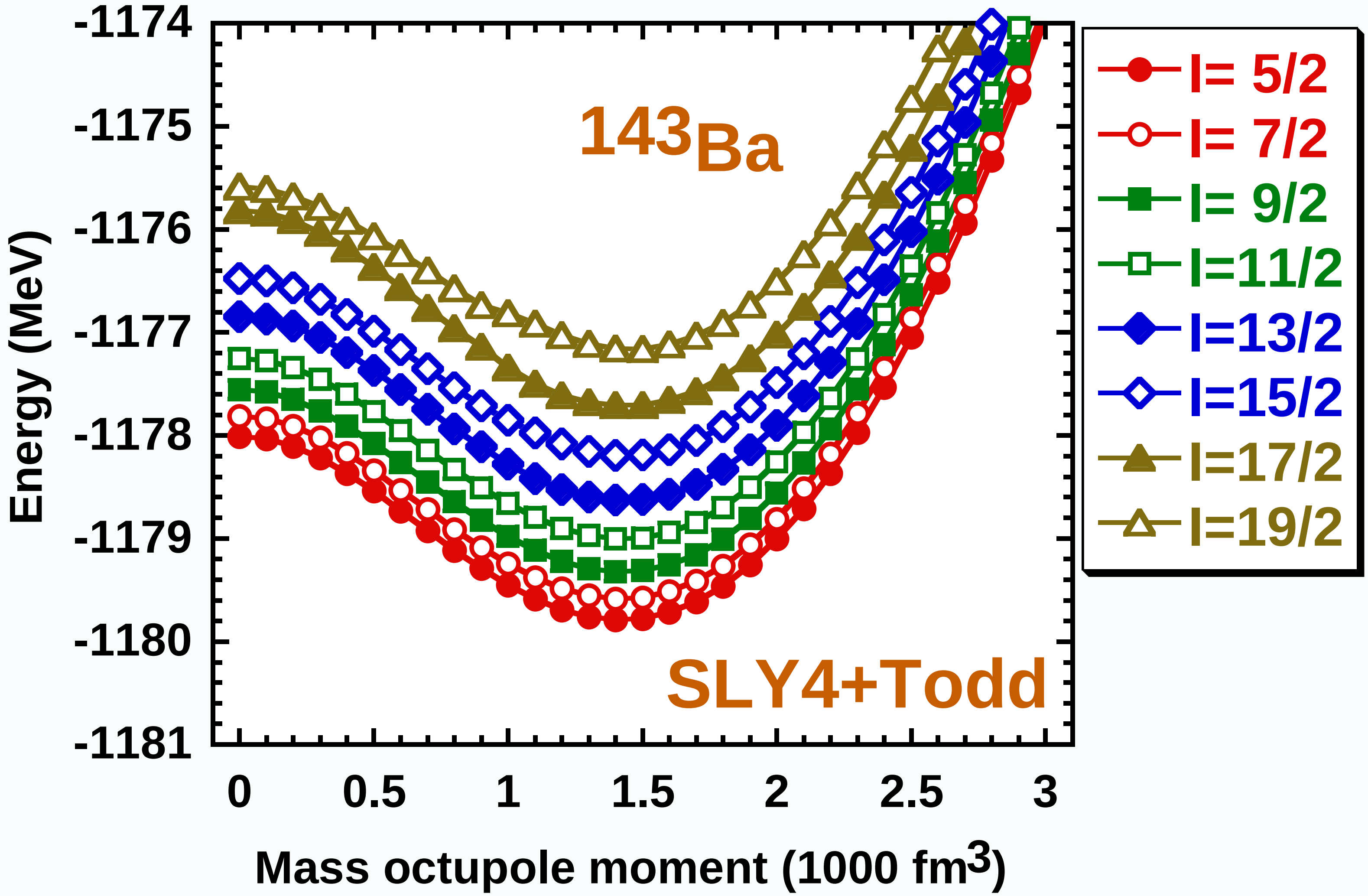
143Ba
D1S
Energy (MeV)
-1165
-1167
-1169
-1171
-1173
-1175
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
I= 5/2
I= 7/2
I= 9/2
I=11/2
I=13/2
I=15/2
I=17/2
I=19/2


D1S
143Ba
I= 5/2
I= 7/2
I= 9/2
I=11/2
I=13/2
I=15/2
I=17/2
I=19/2
Energy (MeV)
0
1
2
3
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)

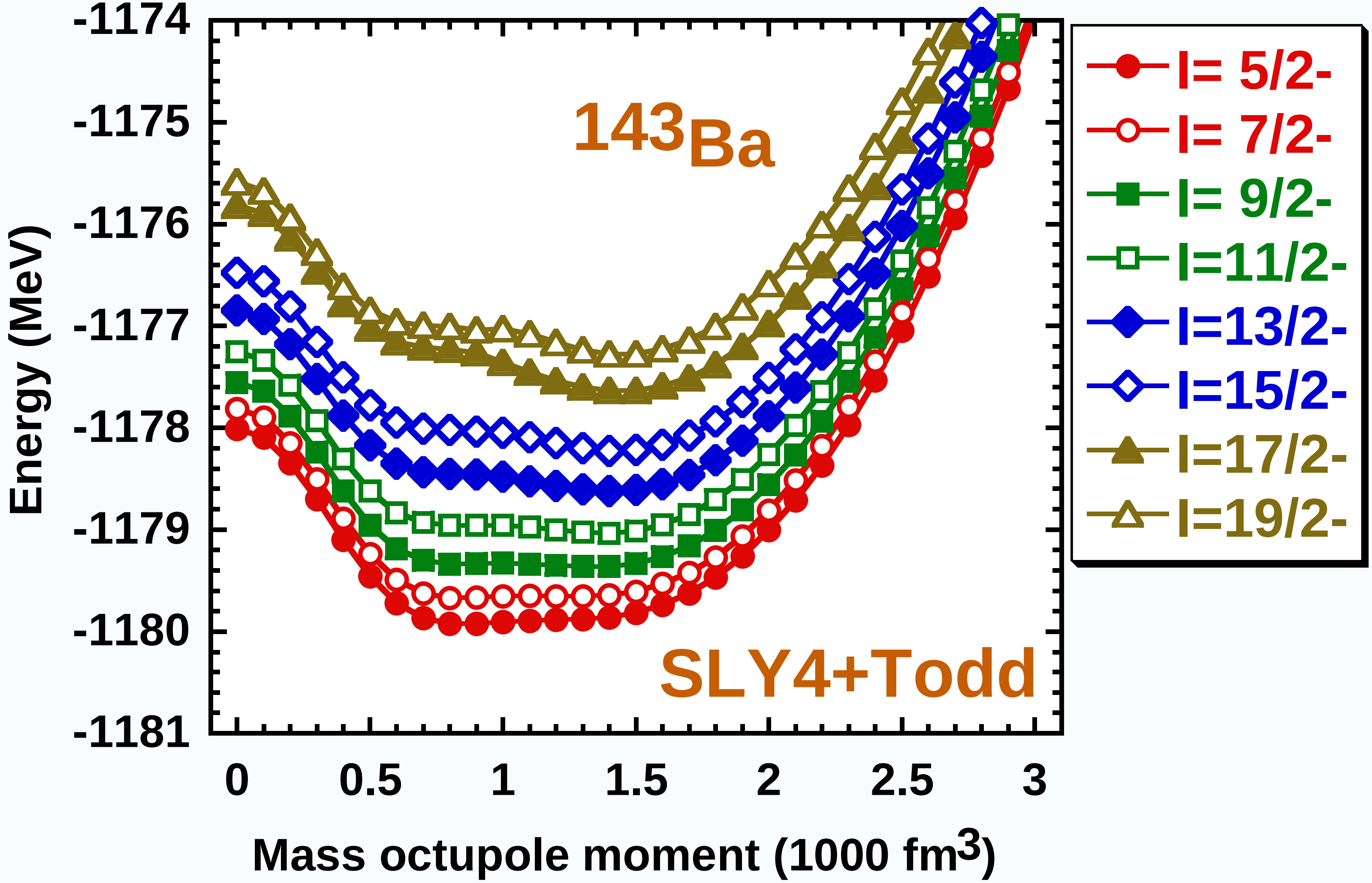

D1S
143Ba
Energy (MeV)
Mass octupole moment (1000 fm3)
0
0.5
1
1.5
2
2.5
3
I= 5/2-
I= 7/2-
I= 9/2-
I=11/2-
I=13/2-
I=15/2-
I=17/2-
I=19/2-



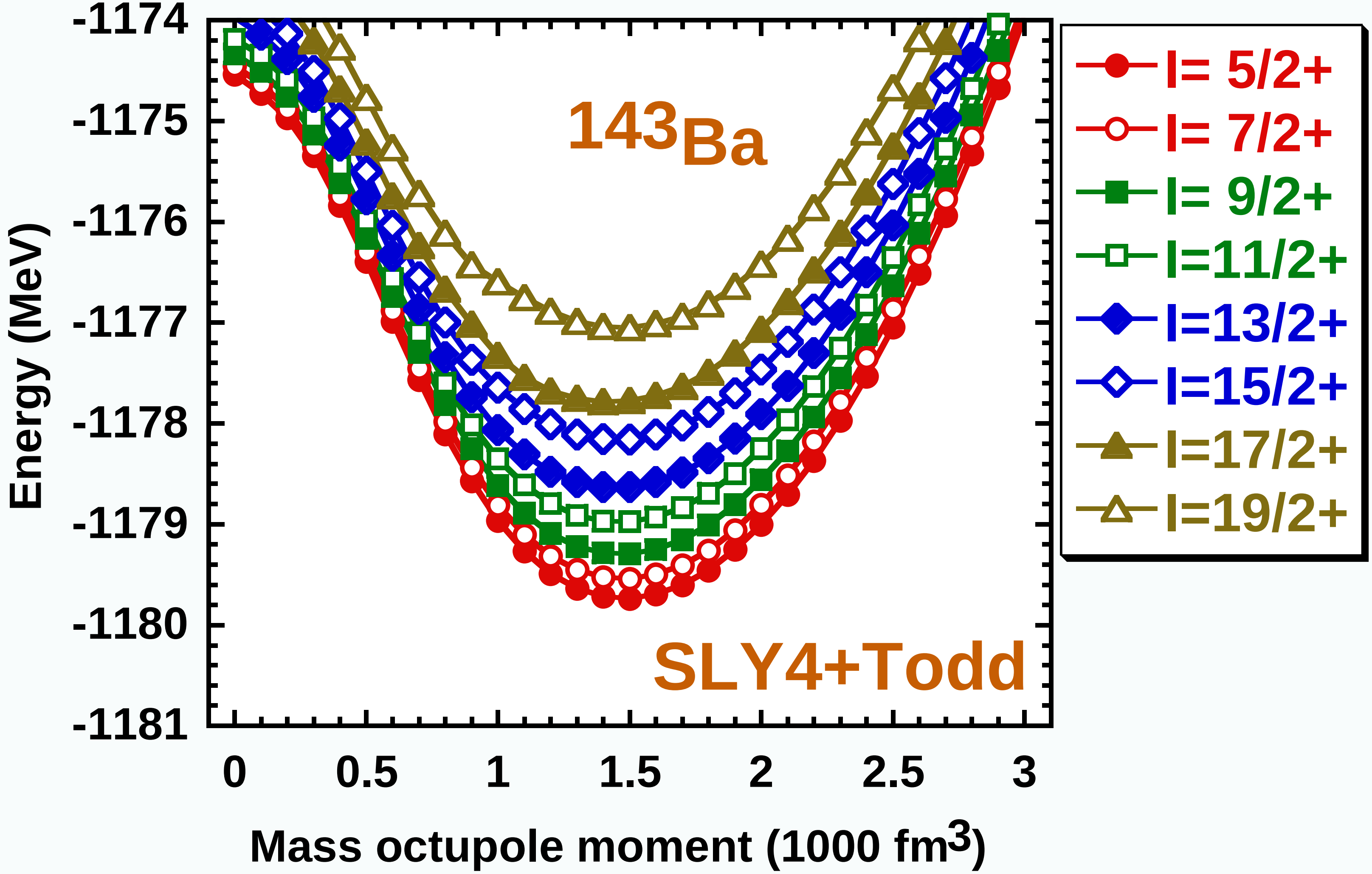
D1S
143Ba
Energy (MeV)
Mass octupole moment (1000 fm3)
I= 5/2+
I= 7/2+
I= 9/2+
I=11/2+
I=13/2+
I=15/2+
I=17/2+
I=19/2+
0
1
2
3
0
0.5
1
1.5
2
2.5
3



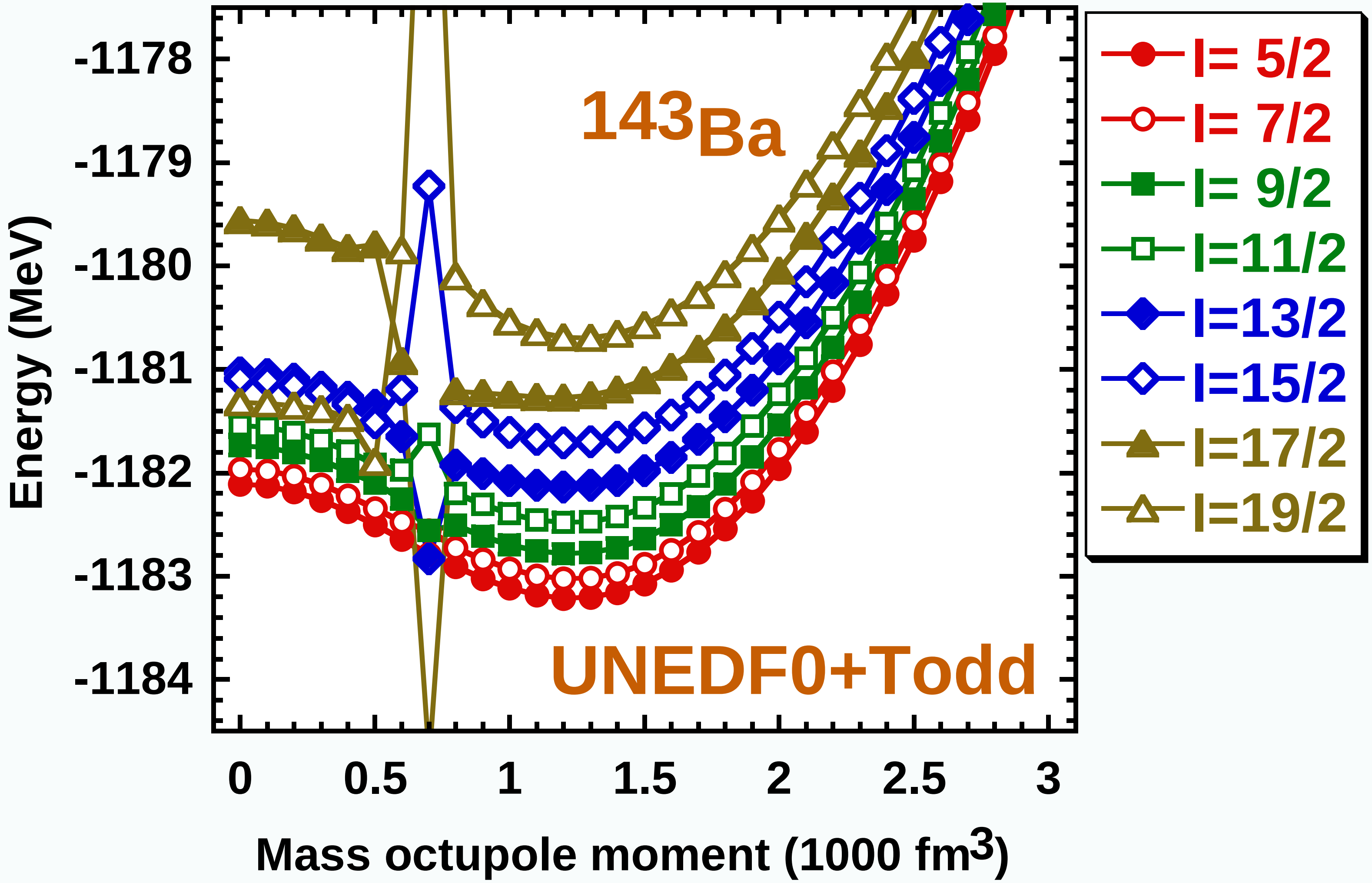
143Ba
SLY4+Todd
Energy (MeV)
Mass octupole moment (1000 fm3)
-1174
-1175
-1176
-1177
-1178
-1179
-1180
-1181
0
0.5
1
1.5
2
2.5
3
I= 5/2
I= 7/2
I= 9/2
I=11/2
I=13/2
I=15/2
I=17/2
I=19/2



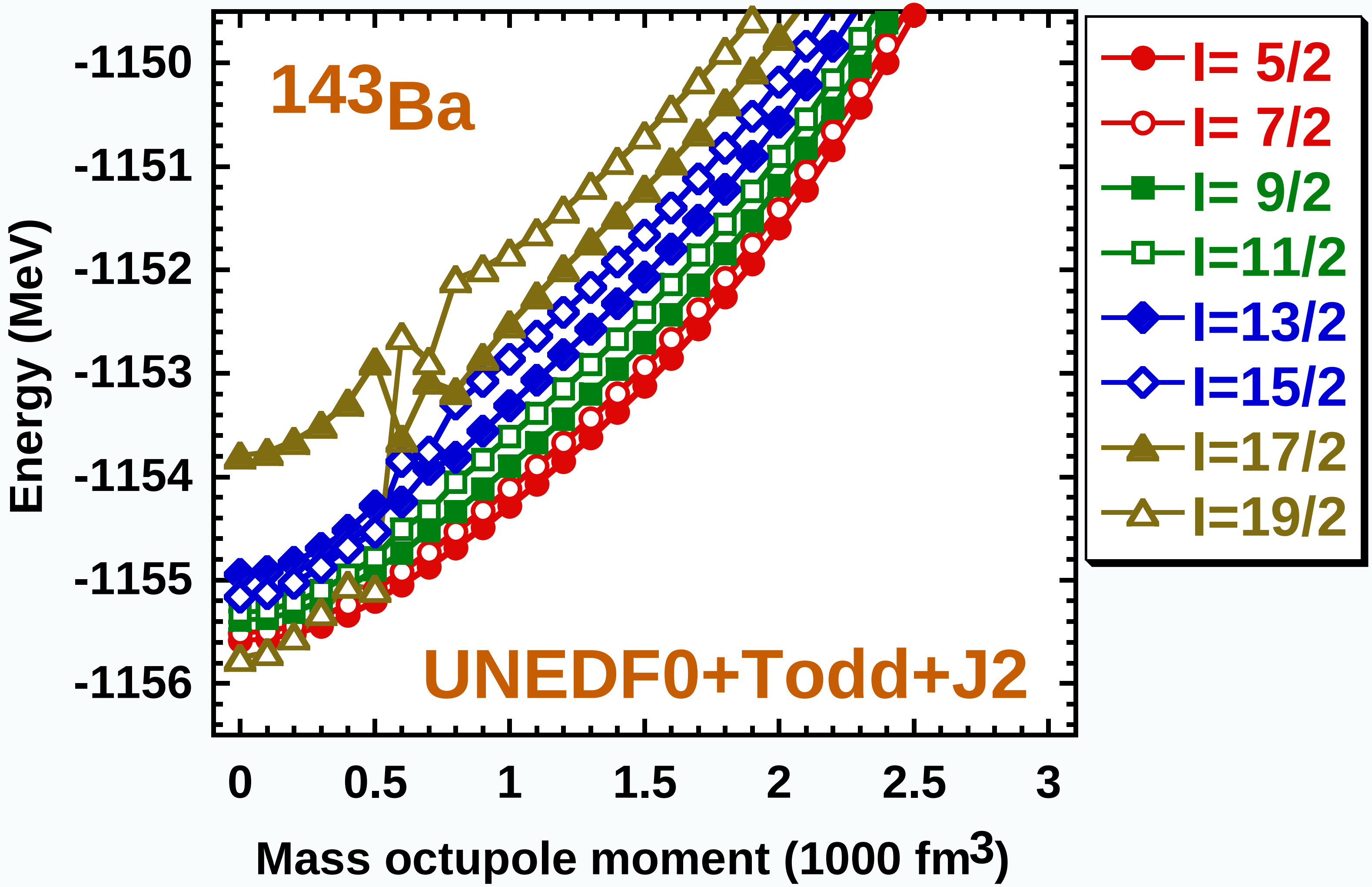
143Ba
SLY4+Todd
Energy (MeV)
-1174
-1175
-1176
-1177
-1178
-1179
-1180
-1181
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
I= 5/2-
I= 7/2-
I= 9/2-
I=11/2-
I=13/2-
I=15/2-
I=17/2-
I=19/2-



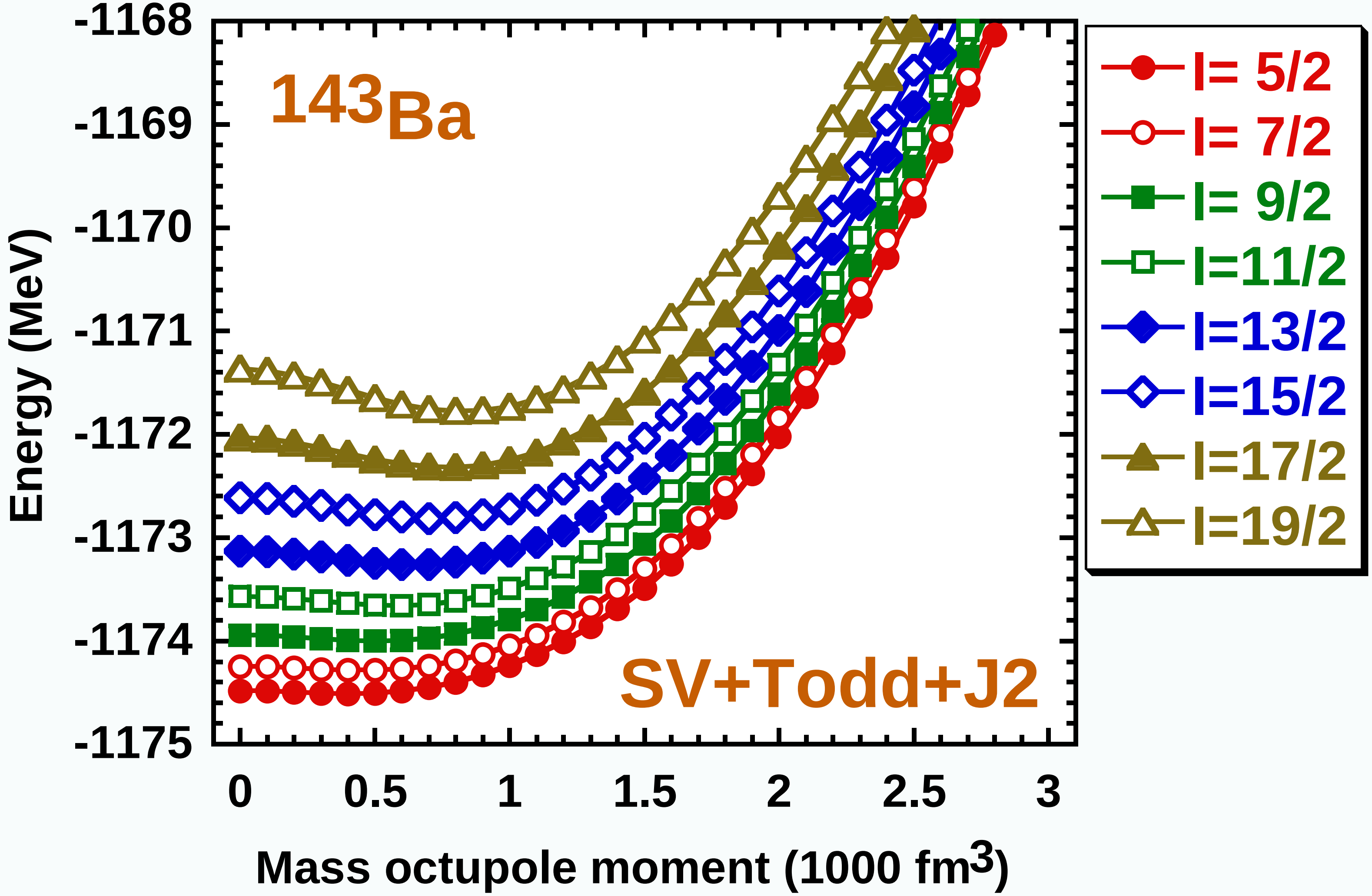
-1174
-1175
-1176
-1177
-1178
-1179
-1180
-1181
Energy (MeV)
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
143Ba
SLY4+Todd
I= 5/2+
I= 7/2+
I= 9/2+
I=11/2+
I=13/2+
I=15/2+
I=17/2+
I=19/2+



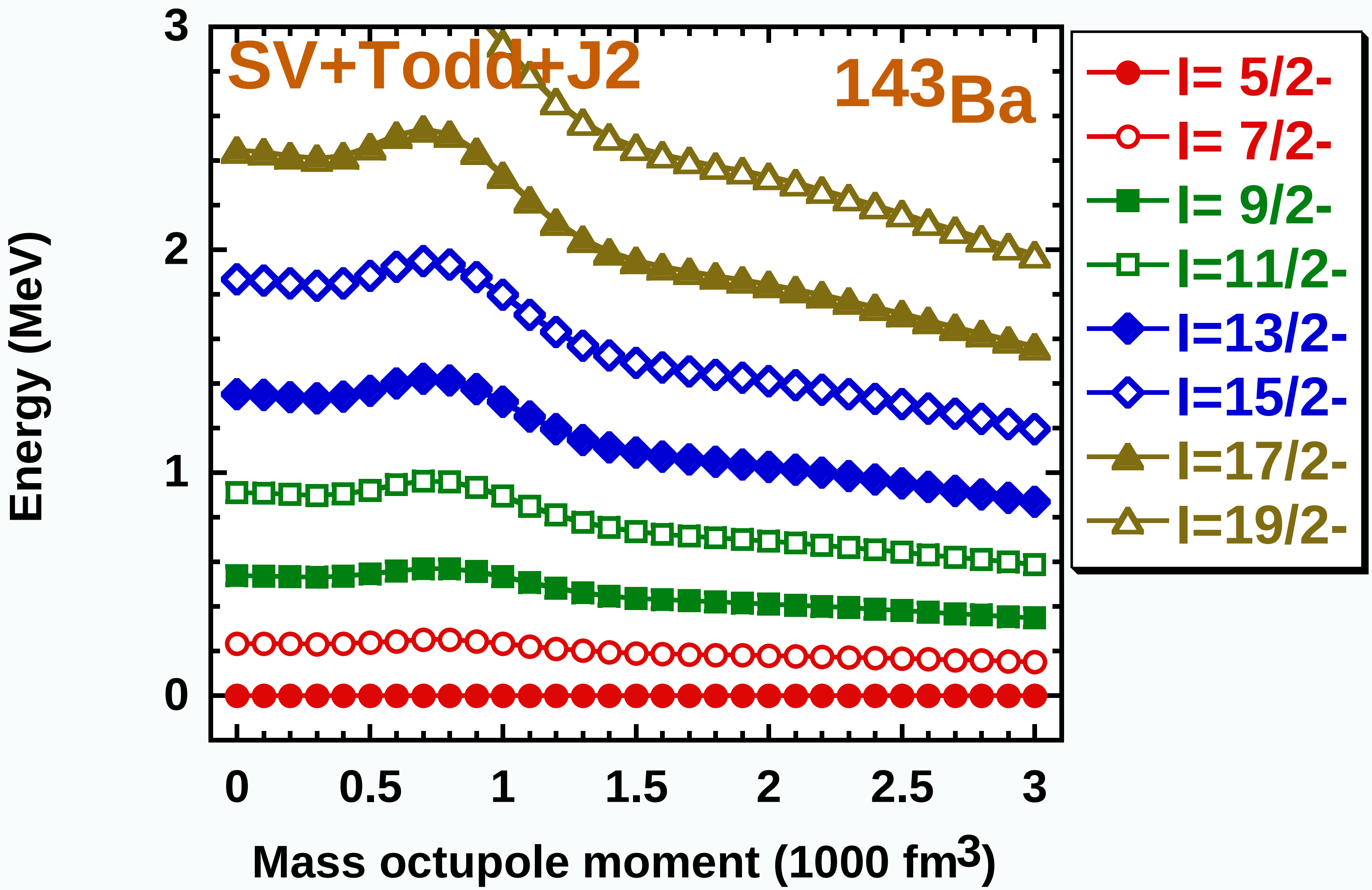
143Ba
UNEDF0+Todd
Energy (MeV)
-1178
-1179
-1180
-1181
-1182
-1183
-1184
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
I= 5/2
I= 7/2
I= 9/2
I=11/2
I=13/2
I=15/2
I=17/2
I=19/2



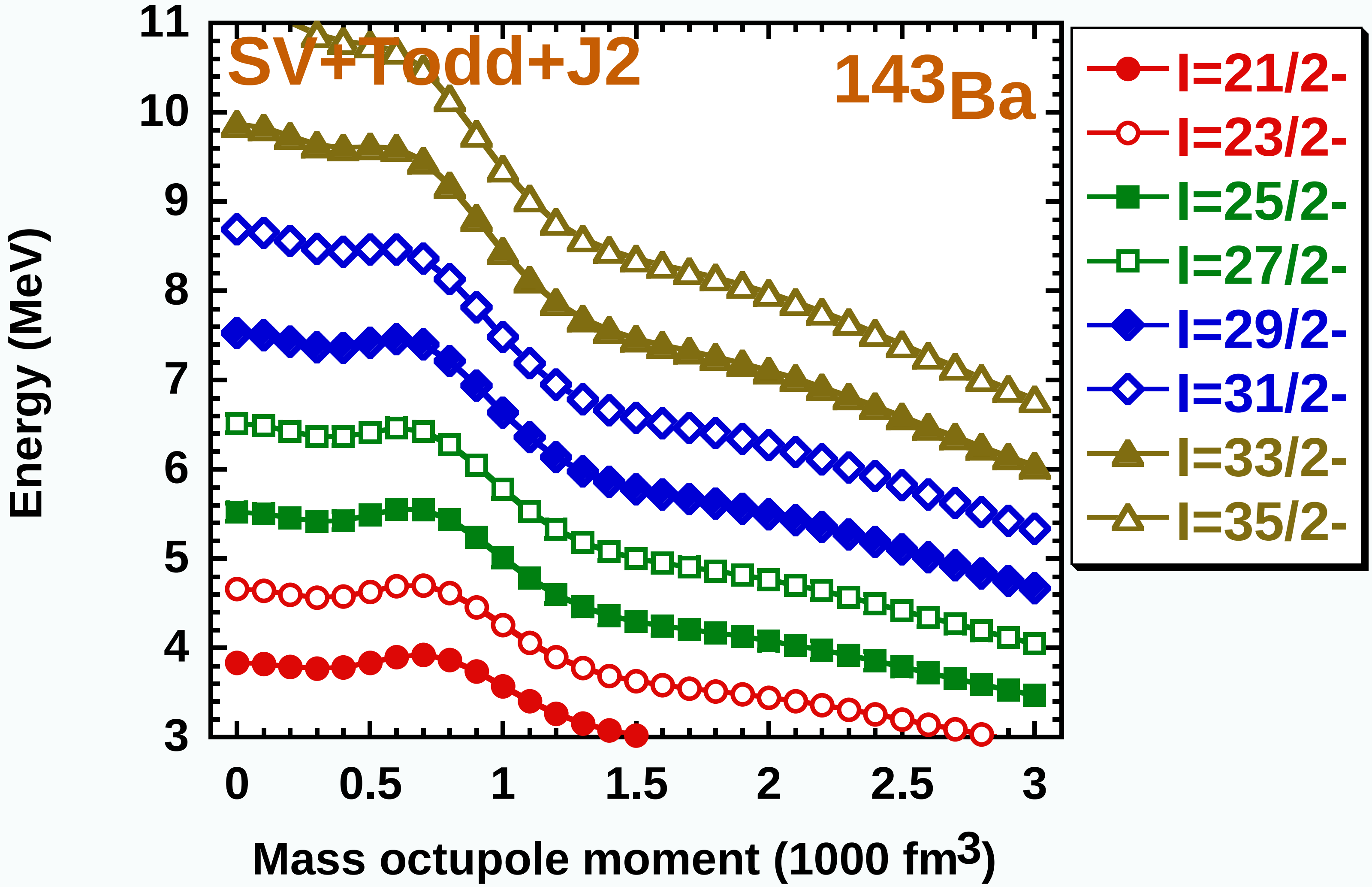
143Ba
UNEDF0+Todd+J2
Energy (MeV)
-1150
-1151
-1152
-1153
-1154
-1155
-1156
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
I= 5/2
I= 7/2
I= 9/2
I=11/2
I=13/2
I=15/2
I=17/2
I=19/2

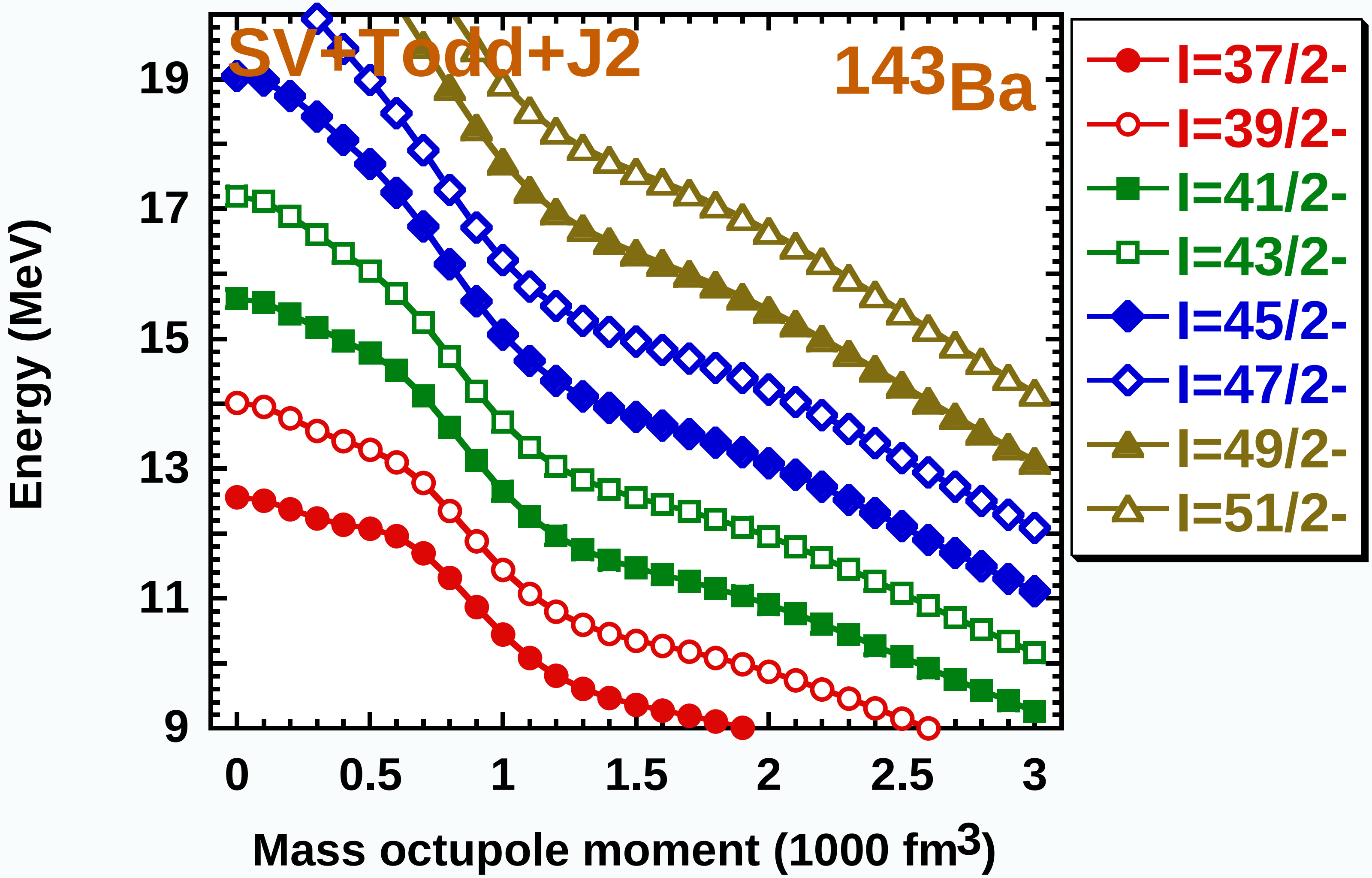


143Ba
SV+Todd+J2
Energy (MeV)
Mass octupole moment (1000 fm3)
-1168
-1169
-1170
-1171
-1172
-1173
-1174
-1175
0
0.5
1
1.5
2
2.5
3
I= 5/2
I= 7/2
I= 9/2
I=11/2
I=13/2
I=15/2
I=17/2
I=19/2



SV+Todd+J2
143Ba
I= 5/2-
I= 7/2-
I= 9/2-
I=11/2-
I=13/2-
I=15/2-
I=17/2-
I=19/2-
Energy (MeV)
Mass octupole moment (1000 fm3)
0
1
2
3
0
0.5
1
1.5
2
2.5
3


SV+Todd+J2
143Ba
11
10
9
8
7
6
5
4
3
Energy (MeV)
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
I=21/2-
I=23/2-
I=25/2-
I=27/2-
I=29/2-
I=31/2-
I=33/2-
I=35/2-


SV+Todd+J2
143Ba
Energy (MeV)
19
17
15
13
11
9
0
0.5
1
1.5
2
2.5
3
Mass octupole moment (1000 fm3)
I=37/2-
I=39/2-
I=41/2-
I=43/2-
I=45/2-
I=47/2-
I=49/2-
I=51/2-

What's next for ^{143}Ba?

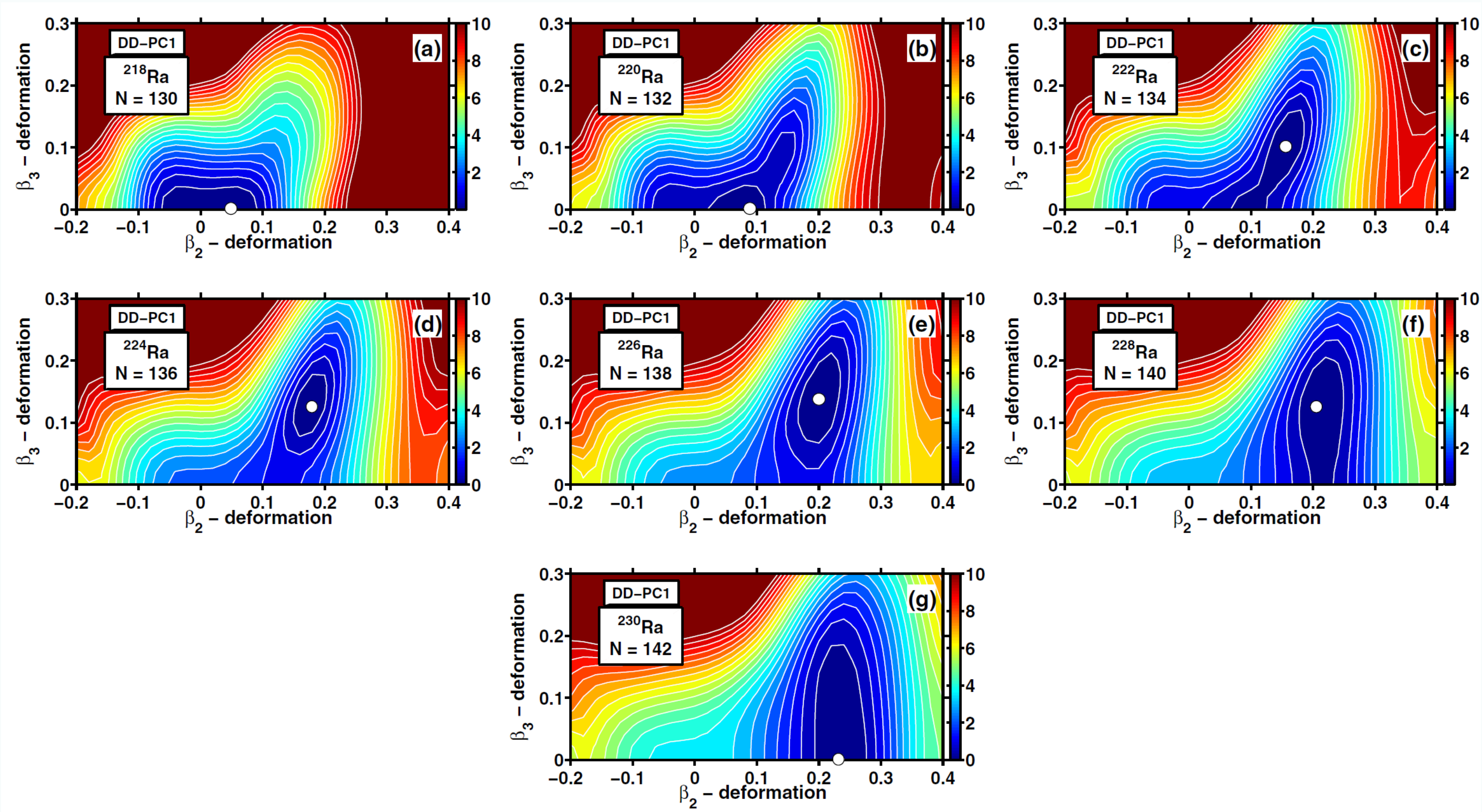
1. Shut your eyes, calculate, publish, drink some beer, and be generally happy.
2. Make some progress once functionals based on the density-independent generators become available.

Conclusions

1. Octupole collectivity in actinides is robustly predicted but imprecisely described.
2. Schiff moments are strongly correlated with octupole moments.
3. Details of structure of individual orbitals are important for the description of ^{229}Th, adjustments to data are mandatory.
4. Description of octupole collectivity is hampered by singularities in angular-momentum restoration.

Thank you

S. E. AGBEMAVA, A. V. AFANASJEV, AND P. RING
PHYSICAL REVIEW C 93, 044304 (2016)



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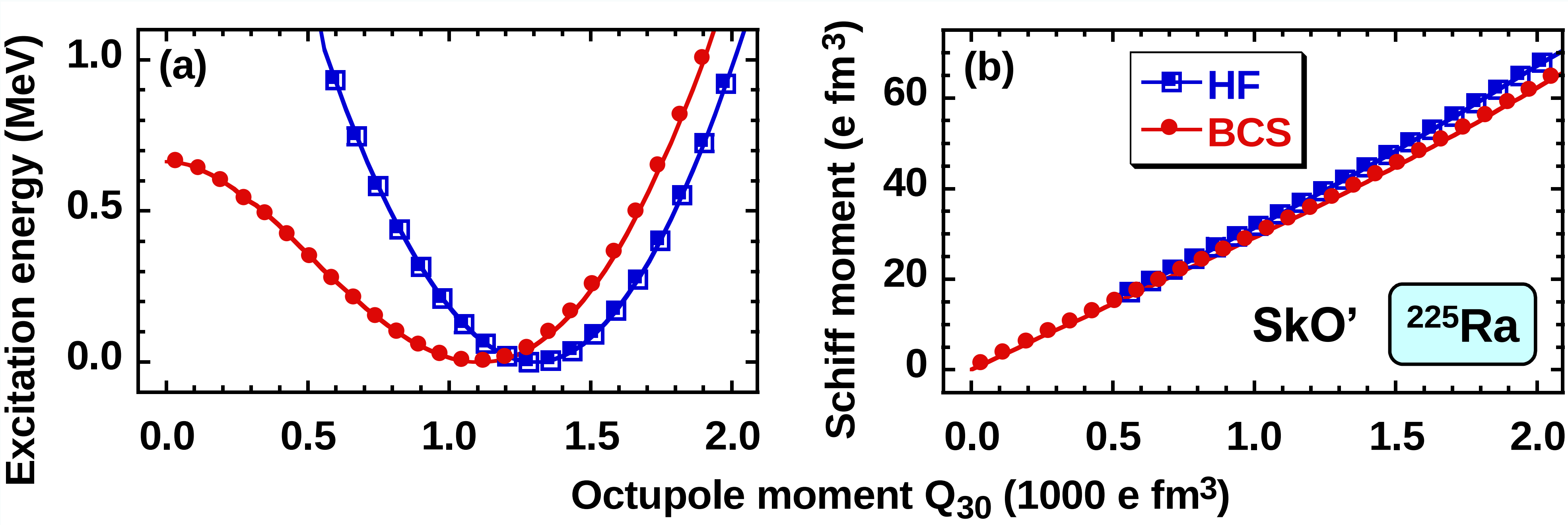
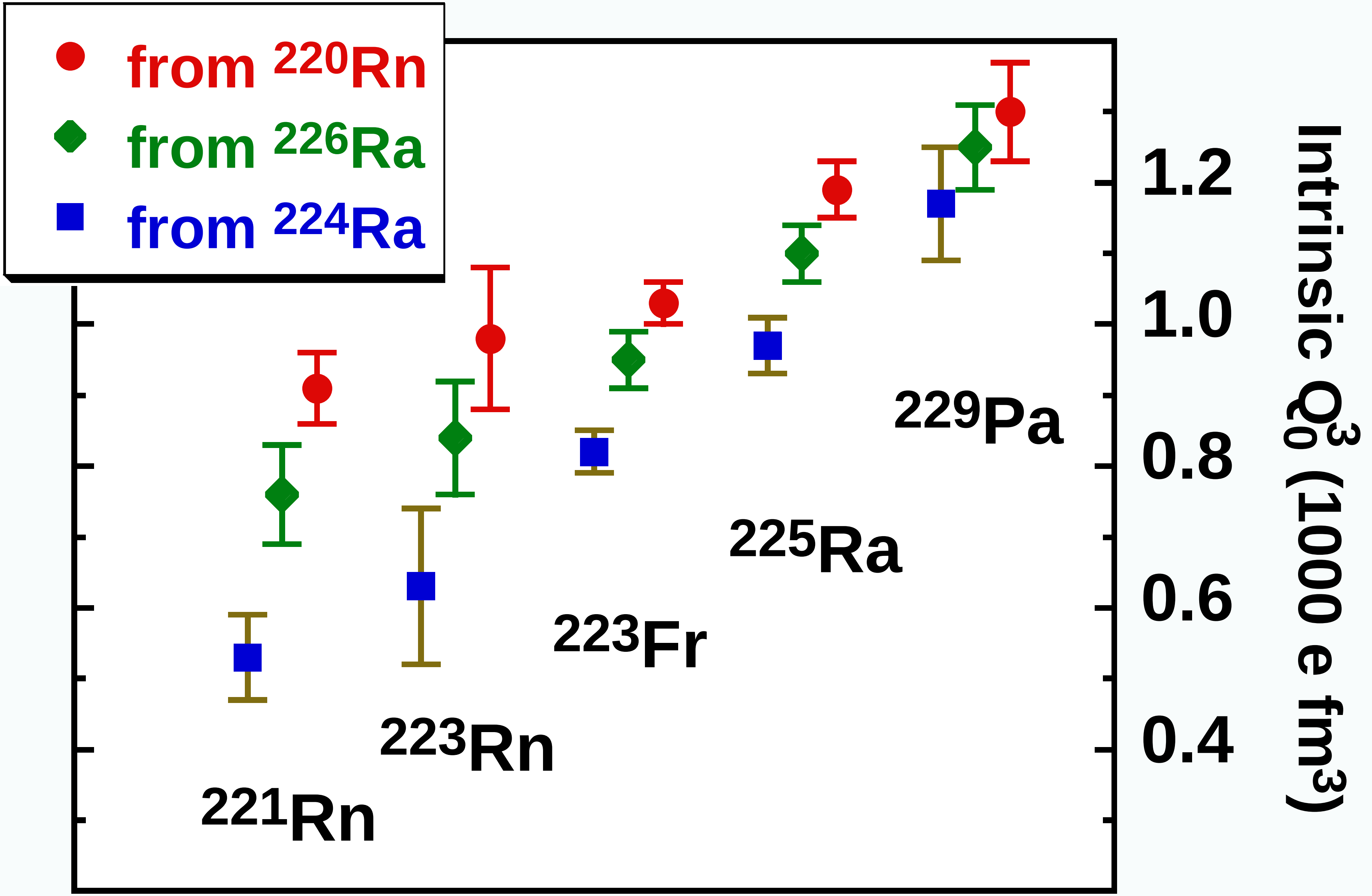
Intrinsic Schiff moments vs. octupole moments



Intrinsic octupole moments in actinides – summary



Laboratory Schiff moments

$$S \equiv \langle \Psi_0 | \hat{S}_0 | \Psi_0 \rangle \approx \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{S}_0 | \Psi_i \rangle \langle \Psi_i | \hat{V}_{PT} | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.}\,,$$

$$S \approx -2 \frac{\langle \Psi_0 | \, \hat{S}_0 \, | \overline{\Psi}_0 \rangle \, \langle \overline{\Psi}_0 | \, \hat{V}_{PT} \, | \Psi_0 \rangle}{\Delta E}$$

$$\langle \Psi_0 | \, \hat{S}_0 \, | \overline{\Psi}_0 \rangle_{\text{rigid}} = \frac{1}{3} S_0,$$

$$\langle \overline{\Psi}_0 | \, \hat{V}_{PT} \, | \Psi_0 \rangle_{\text{rigid}} = \langle \hat{V}_{PT} \rangle$$

$$S = a_0 \, g \, \bar{g}_0 + a_1 \, g \, \bar{g}_1 + a_2 \, g \, \bar{g}_2$$

NucMagMom Collaboration (est. 2017)

- Michael Bender, Lyon
- Witek Nazarewicz, Mengzhi Chen, MSU
- Alessandro Pastore, Pierre Becker, York
- .... all wishing to join are welcome

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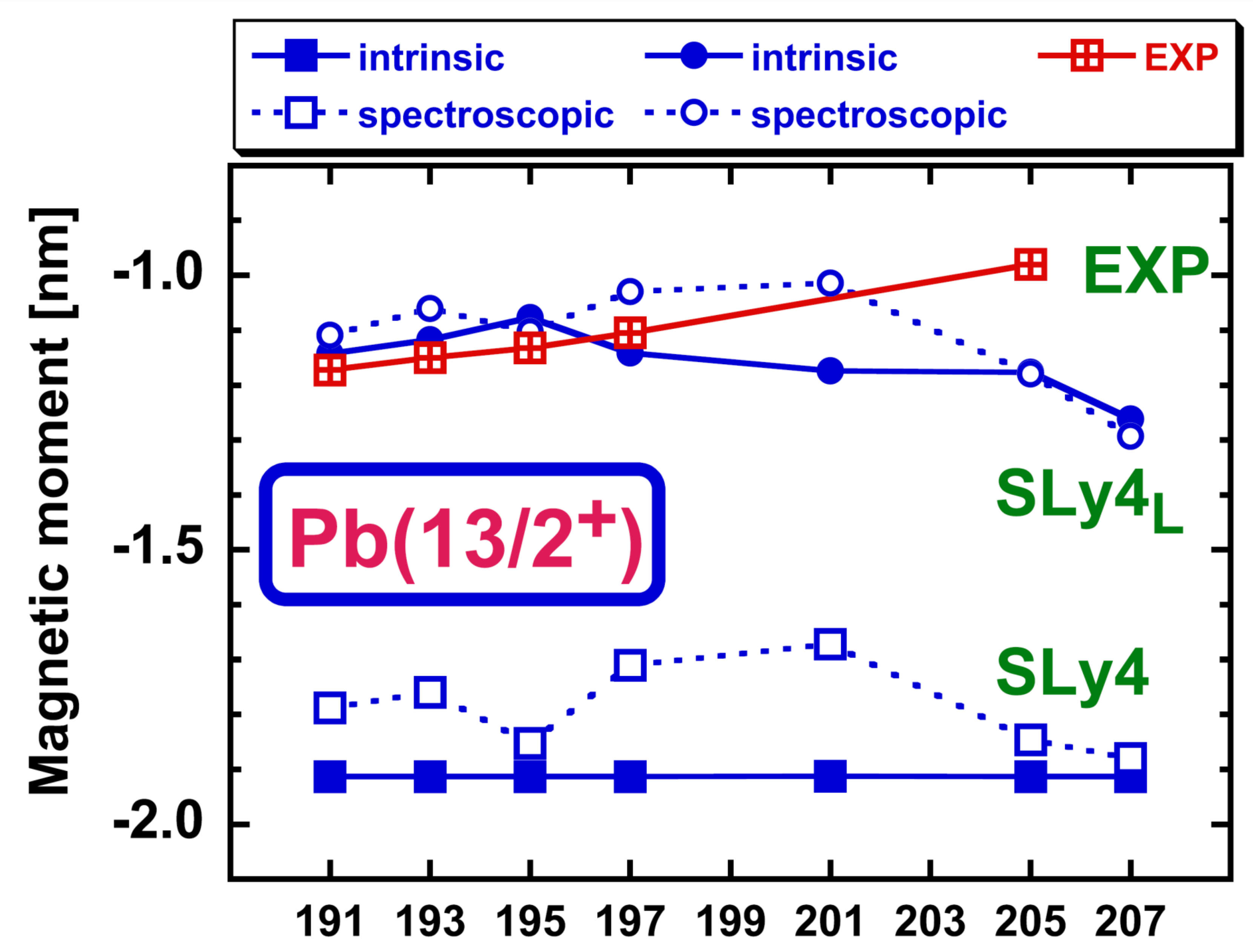
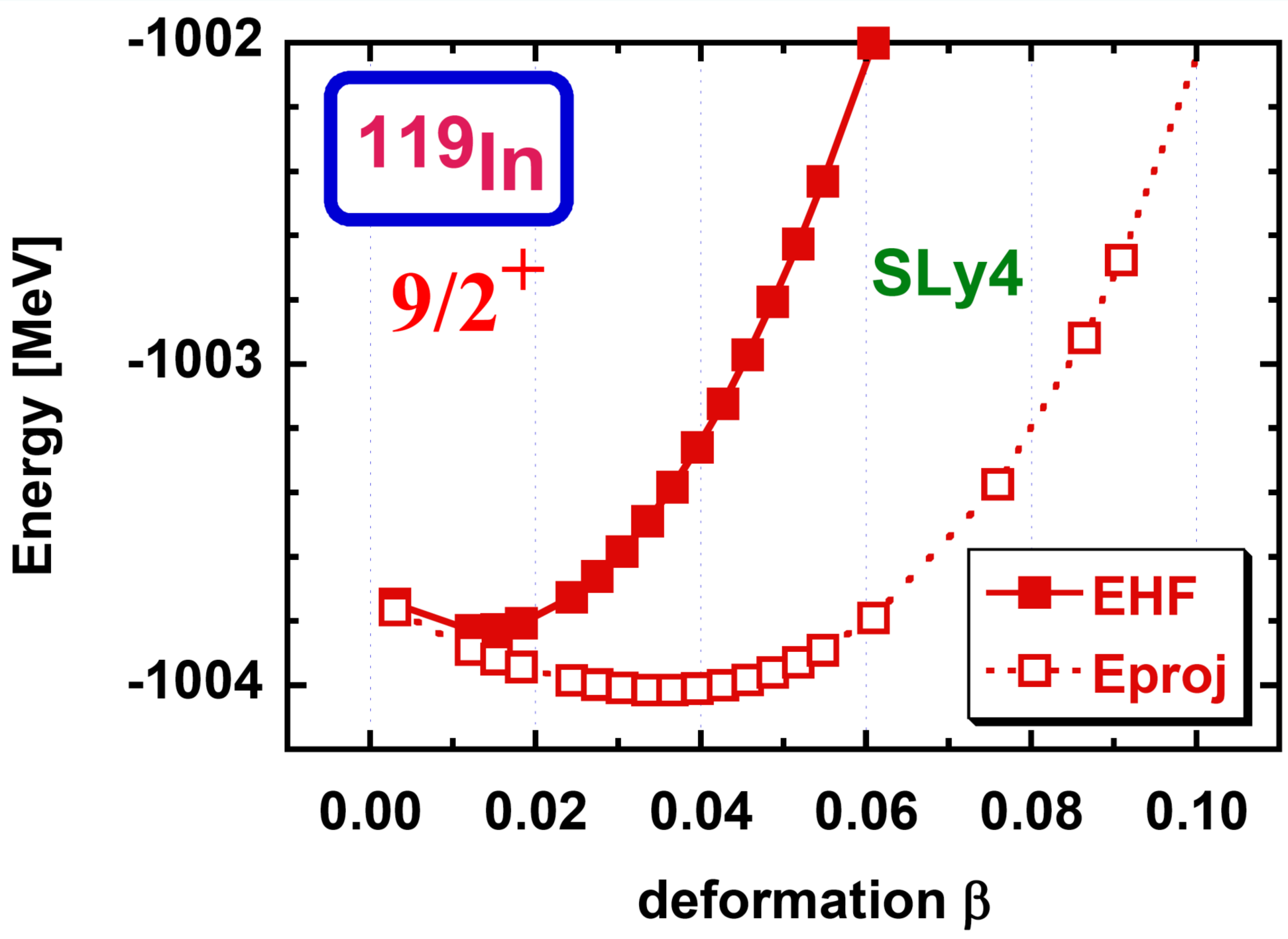
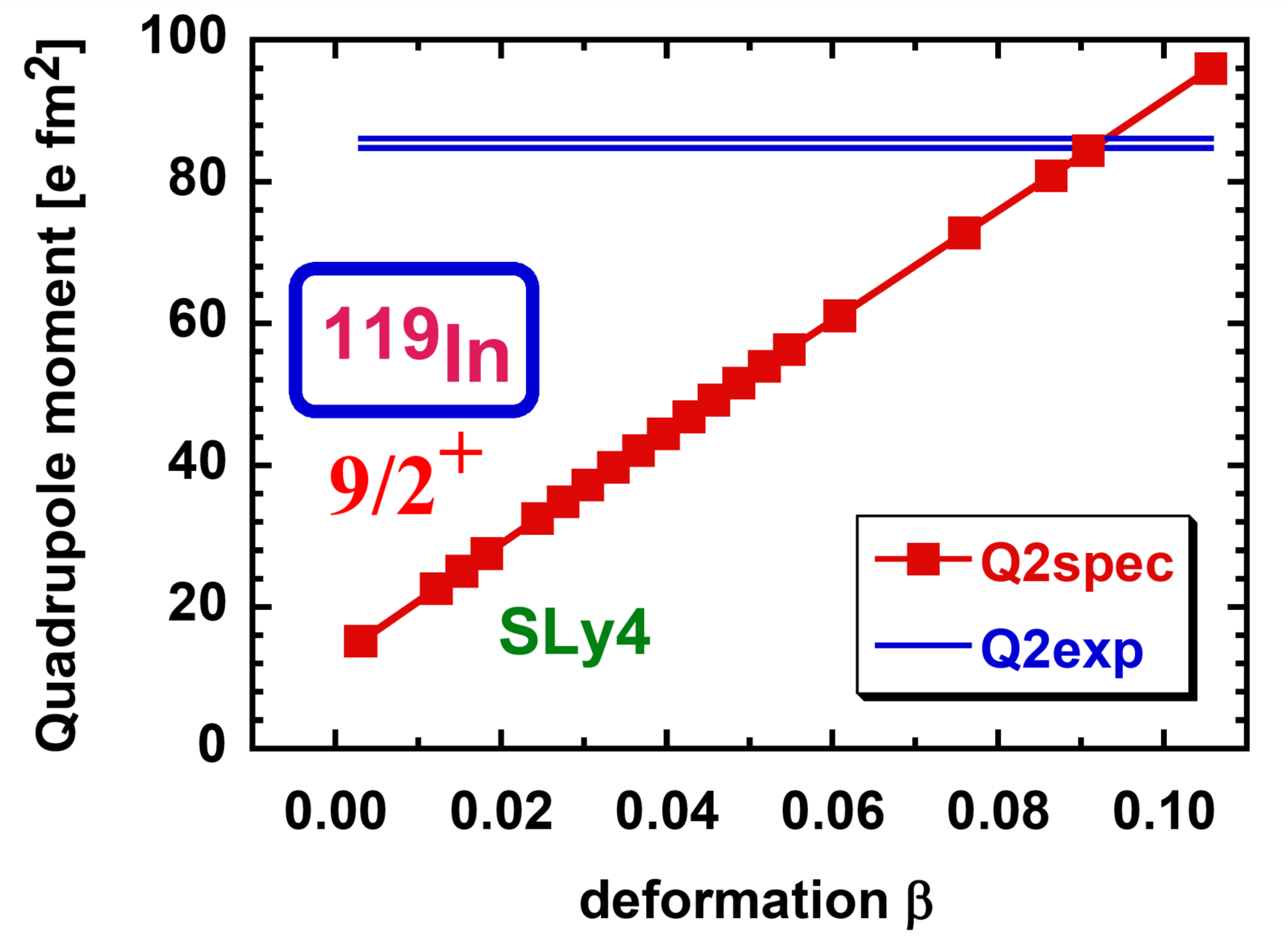
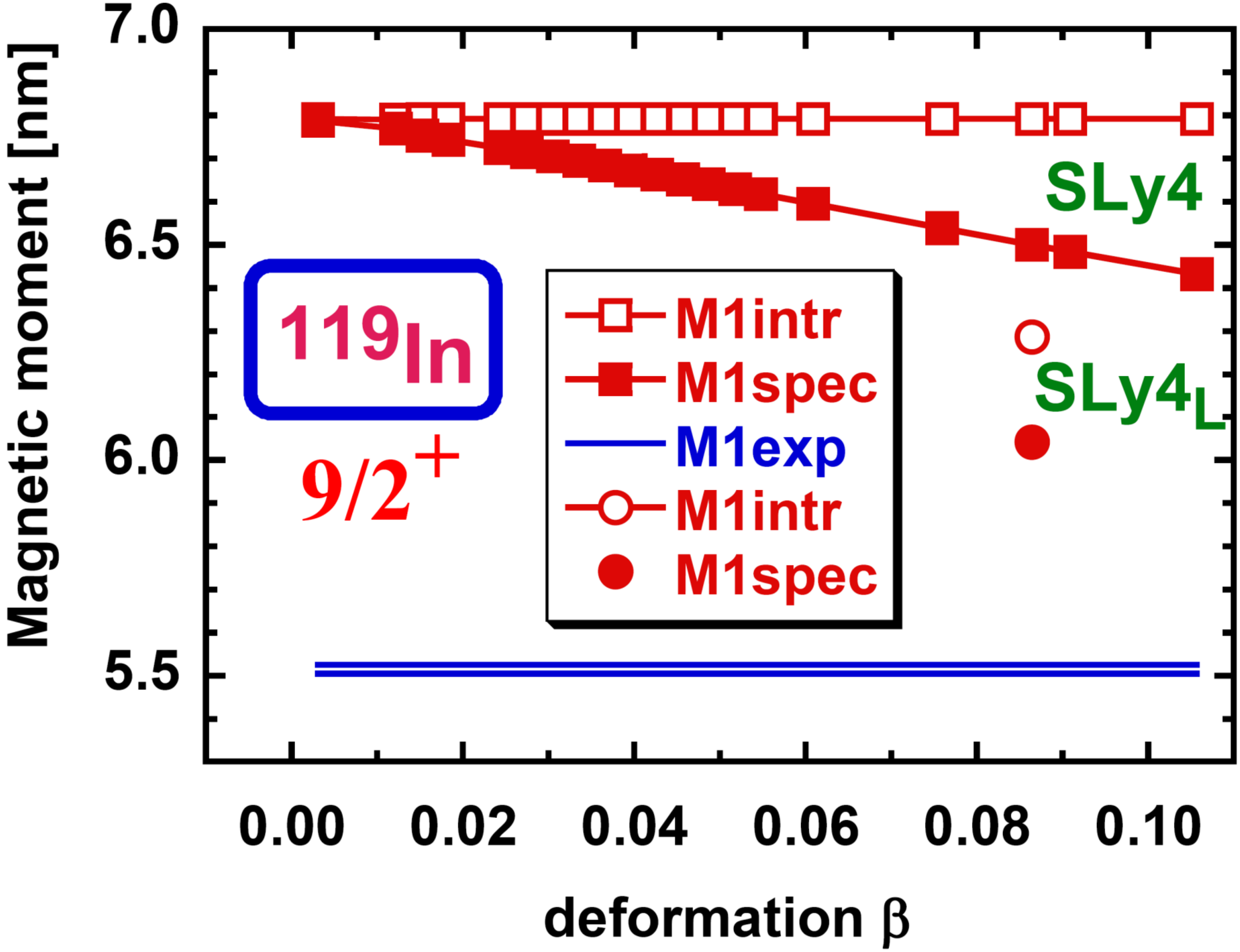


intrinsic
spectroscopic
intrinsic
spectroscopic
EXP
Magnetic moment [nm]
-1.0
-1.5
-2.0
191
193
195
197
199
201
203
205
207
EXP
SLy4L
Pb(13/2+)
SLy4


119In
9/2+
SLy4
EHF
Eproj
-1002
-1003
-1004
Energy [MeV]
0.00
0.02
0.04
0.06
0.08
0.10
deformation β


Quadrupole moment [e fm^2]
100
80
60
40
20
0
0.00
0.02
0.04
0.06
0.08
0.10
deformation β
^{119}In
9/2$^+$
SLy4
Q2spec
Q2exp


Magnetic moment [nm]
7.0
6.5
6.0
5.5
0.00
0.02
0.04
0.06
0.08
0.10
deformation β
119In
9/2+
M1intr
M1spec
M1exp
M1intr
M1spec
SLy4
SLy4L