Nuclear shape effects at the border of atomic energy scale

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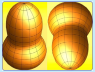

QPTN9, Padova 22 May 2018

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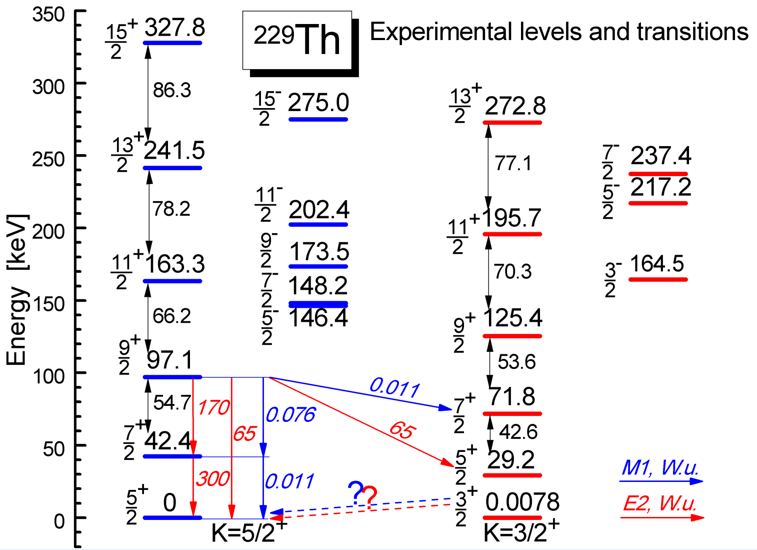
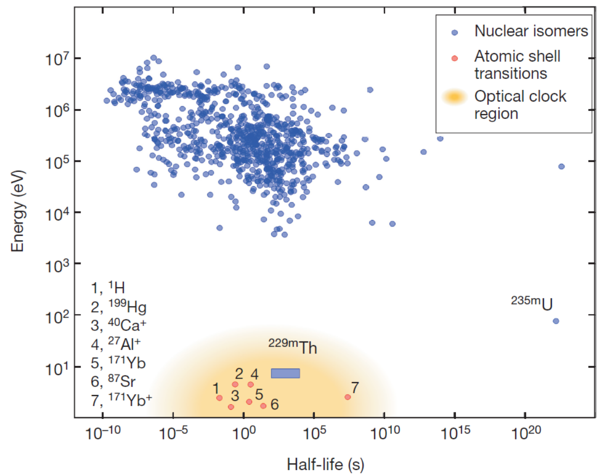
^{229}Th: Low-energy levels and transitions

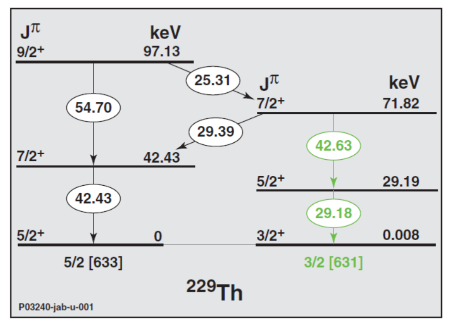


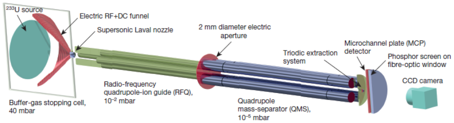
Energy-half-life distribution



L. von der Wense *et al.*, Nature **533**, 47 (2016)

^{229}Th, $3/2^+$ isomer: energy estimates and decay detection





L. Kroger, C. Reich, NPA **259**, 29 (1976), $E(^{229m}Th) < 100$eV
D.Burke et al, PRC1990,NPA2008
R. Helmer, C. Reich, PRC **49**, 1845 (1994), $E(^{229m}Th) \sim 3.5$eV
Last energy estimate:
$E(^{229m}Th) =$
$(29.39 - 29.18) - (42.63 - 42.43)$
~ 0.0078 keV
B. Beck et al, PRL **98**, 142501 (2007); LLNL-PROC-415170 (2009)

Decay detection:
L. von Wense et al, Nature **533**, 47 (2016), $\tau\ (^{229m}\mathrm{Th}^{2+}) \gtrsim 60$s
B. Seiferle et al, PRL **118**, 042501 (2017), $\tau\ (^{229m}\mathrm{Th})\ 7 \pm 1\mu$s

^{229}Th: $3/2^+$ isomer possible applications

✓ Phenomena on the border between nuclear and atomic physics
✓ Nuclear quantum optics with X-ray laser pulses [T. Bürvenich et al., PRL **96**, 142501 (2006)]
✓ Nuclear γ-ray laser of optical range [E. Tkalya, PRL **106**, 162501 (2011)]
✓ Nuclear clock with a total fractional inaccuracy approaching $1 \times 10^{-19} - 10^{-20}$ outperforming the existing atomic-clock technology [C. J. Campbell et al., PRL **108**, 120802 (2012)]
✓ ⇒ Investigation of possible time variations of fundamental constants (fine structure constant $\alpha = e^2/\hbar c$; strong interaction parameter $m_q/\Lambda_{\mathrm{QCD}}$): Unification theories → cosmology → variation of the fundamental constants in the expanding Universe (quasar absorption spectra, big bang nucleosynthesis) [V. V. Flambaum, PRL **97**, 092502 (2006)]

Quadrupole-octupole core plus particle Hamiltonian

$$H = H_{\mathrm{qo}} + H_{\mathrm{s.p.}} + H_{\mathrm{pair}} + H_{\mathrm{Coriol}}$$

$$H_{\mathrm{qo}} = -\frac{\hbar^2}{2B_2}\frac{\partial^2}{\partial\beta_2^2} - \frac{\hbar^2}{2B_3}\frac{\partial^2}{\partial\beta_3^2} + U(\beta_2,\beta_3,I)$$

$$U(\beta_2,\beta_3,I) = \frac{1}{2}C_2{\beta_2}^2 + \frac{1}{2}C_3{\beta_3}^2 + \frac{d_0 + \hat{I}^2 - {\hat{I}_z}^2}{2\mathcal{J}(\beta_2,\beta_3)}$$

$$H_{\mathrm{Coriol}} = -\frac{(\hat{I}_+\hat{j}_- + \hat{I}_-\hat{j}_+)}{2\mathcal{J}(\beta_2,\beta_3)}, \qquad \mathcal{J}(\beta_2,\beta_3) = (d_2\beta_2^2 + d_3\beta_3^2)$$

$$H_{\mathrm{sp}} = T + V_{\mathrm{ws}}(\beta_2,\beta_3,\ldots) + V_{\mathrm{s.o.}} + V_{\mathrm{c}}$$

$$H_{qp} \equiv H_{\mathrm{s.p.}} + H_{\mathrm{pair}} \rightarrow \epsilon^K_{\mathrm{qp}} = \sqrt{(E^K_{\mathrm{sp}} - \lambda)^2 + \Delta^2}$$

Coherent quadrupole-octupole mode (CQOM) in the even core

$$U(\beta_2,\beta_3,I)+\langle H_{\text{Coriol}}\rangle=\frac{1}{2}C_2{\beta_2}^2+\frac{1}{2}C_3{\beta_3}^2+\frac{\widetilde{X}(I,K)}{d_2\beta_2^2+d_3\beta_3^2}$$

$$\widetilde{X}(I,K)=[d_0+I(I+1)-K^2+2\mathcal{J}\langle H_K^c\rangle]/2$$

$$\beta_2=\sqrt{d/d_2}\eta\cos\phi\ ,\quad \beta_3=\sqrt{d/d_3}\eta\sin\phi\ ,\quad d=(d_2+d_3)/2$$

Coherent mode: $\omega=\sqrt{C_2/B_2}=\sqrt{C_3/B_3}\equiv\sqrt{C/B}$

$H_{\text{qo}}+H_{\text{Coriol}}$ → **energy spectrum:**

$$E_{n,k}(I,K)=\hbar\omega\left[2n+1+\sqrt{k^2+b\widetilde{X}(I,K)}\right],\quad n=0,1,2,...$$

Quadrupole-octupole vibration function of the core

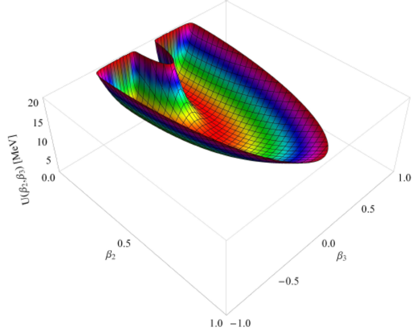
$$\Phi^{\pi}_{n,k,I}(\eta,\phi) = \psi^{I}_{nk}(\eta)\varphi^{\pi}_{k}(\phi)$$

$$\psi^{I}_{nk}(\eta) = \sqrt{\frac{2c\Gamma(n+1)}{\Gamma(n+2s+1)}}e^{-c\eta^2/2}c^s\eta^{2s}L^{2s}_{n}(c\eta^2)$$

$$\begin{aligned}\varphi^{+}_{k}(\phi) &= \sqrt{2/\pi}\cos(k\phi)\ , \quad k=1,3,5,\ldots \\ \varphi^{-}_{k}(\phi) &= \sqrt{2/\pi}\sin(k\phi)\ , \quad k=2,4,6,\ldots\end{aligned}$$

[N. M. et al, Phys. Rev. C **73**, 044315 (2006); **76**, 034324 (2007)]

Quadrupole-octupole potential and the coherent mode



Quadrupole-octupole vibration

Quadrupole-octupole vibration and rotation

Total core plus particle wave function

$$\begin{aligned}\Psi^{\pi,\pi^b}_{nkIMK}(\eta,\phi) &= \frac{1}{2}\sqrt{\frac{2I+1}{16\pi^2}}\,\Phi^{\pi\cdot\pi^b}_{nkI}(\eta,\phi) \\ &\times \left[D^I_{M\,K}(\theta)\mathcal{F}^{(\pi^b)}_{K} + \pi\cdot\pi^b(-1)^{I+K}D^I_{M\,-K}(\theta)\mathcal{F}^{(\pi^b)}_{-K}\right]\end{aligned}$$

$$\widetilde{\Psi}^{\pi,\pi^b}_{nkIMK_b} = \frac{1}{\widetilde{N}_{I\pi K_b}}\left[\Psi^{\pi,\pi^b}_{nkIMK_b} + A \sum_{\substack{\nu\neq b \\ (K_\nu = K_b\pm 1,\frac{1}{2})}} \frac{\widetilde{a}^{(\pi\pi^b)}_{K_\nu K_b}(I)}{\epsilon^{K_\nu} - \epsilon^{K_b}}\Psi^{\pi,\pi^b}_{nkIMK_\nu}\right]$$

$A \equiv 1/[2\mathcal{J}(\beta_2^0,\beta_3^0)] \rightarrow$ K- mixing constant

$\widetilde{a}^{(\pi,\pi^b)}_{K_\nu K_b}(I) \rightarrow$ Coriolis mixing factors $\sim \langle\mathcal{F}^{(\pi^b)}_{K_{\nu'}}|\hat{j}_+|\mathcal{F}^{(\pi^b)}_{K_\nu}\rangle$ from DSM

Quasi parity-doublet spectrum from CQOM+DSM+BCS

$$E_{nk}(I^\pi, K_b) = \epsilon^{K_b}_{\mathbf{qp}} + \hbar\omega \left[2n+1+\sqrt{k^2 + b\widetilde{X}(I^\pi, K_b)}\right]$$

$$\begin{aligned}\widetilde{X}(I^\pi, K_b) \quad &= \quad \frac{1}{2}\Bigg[d_0 + I(I+1) - K_b^2 + (-1)^{I+\frac{1}{2}}\left(I+\frac{1}{2}\right) a^{(\pi\pi^b)}_{\frac{1}{2}}\delta_{K_b,\frac{1}{2}} \\ &- \quad A \sum_{\substack{\nu\neq b \\ (K_\nu = K_b \pm 1, \frac{1}{2})}} \frac{\left[\widetilde{a}^{(\pi\pi^b)}_{K_\nu K_b}(I)\right]^2}{\epsilon^{K_\nu} - \epsilon^{K_b}}\Bigg]\end{aligned}$$

$a^{(\pi,\pi^b)}_{1/2} = \pi\pi_b a^{(\pi^b)}_{\frac{1}{2}-\frac{1}{2}}$ → decoupling factor

[N. M., Phys. Scripta **T154**, 014017 (2013)]

Reduced $E\lambda$ (λ=1,2,3) and $M1$ transition probabilities

$$B(E\lambda;\pi^{b_i} n_i k_i I_i K_i \to \pi^{b_f} n_f k_f I_f K_f) = \frac{1}{2I_i+1}\sum_{M_i M_f \mu}\left|\left\langle \widetilde{\Psi}^{\pi_f,\pi^{b_f}}_{n_f k_f I_f M_f K_f}\right|\hat{\mathcal{M}}_{\mu}(E\lambda)\left|\widetilde{\Psi}^{\pi_i,\pi^{b_i}}_{n_i k_i I_i M_i K_i}\right\rangle\right|^2$$

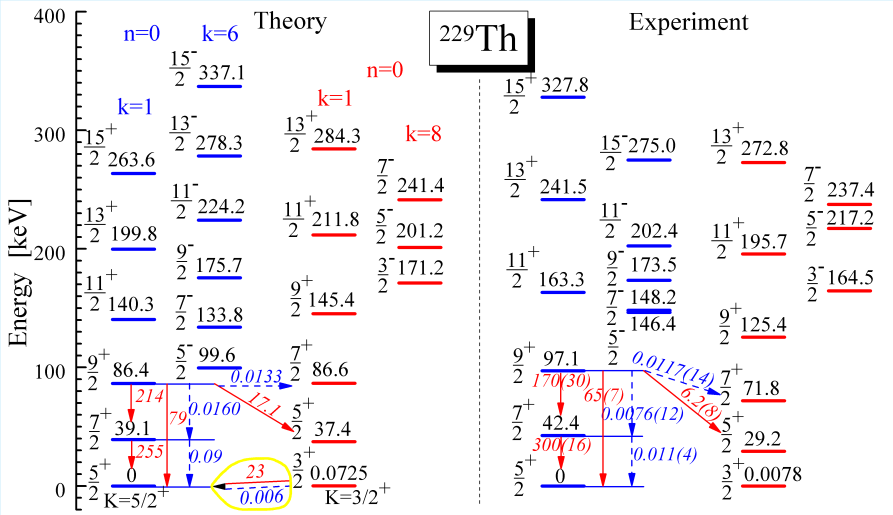
$$\begin{aligned}\langle \mathcal{F}^{(\pi^{b_f})}_{K_f}|\hat{M}1_z|\mathcal{F}^{(\pi^{b_i})}_{K_i}\rangle &= \sqrt{\frac{3}{4\pi}}\mu_N\Big[(g_l-g_R)K_i\delta_{K_f K_i}\langle \mathcal{F}^{(\pi^{b_f})}_{K_f}|\mathcal{F}^{(\pi^{b_i})}_{K_i}\rangle \\ &+ (g_s-g_l)\langle \mathcal{F}^{(\pi^{b_f})}_{K_f}|\hat{s}_z|\mathcal{F}^{(\pi^{b_i})}_{K_i}\rangle\Big]\end{aligned}$$

Coriolis K-mixed matrix elements ⇒ permission of gamma transitions with $K_f \neq K_i$ (forbidden by the axial symmetry)

Details of the CQOM+DSM+BCS model calculations

- General: 2 quasi parity-doublets with identical quantum numbers $n = 0$ and $k^+ = 1$ with $k^- = 2$, or 4, ... built on quasi-degenerate 5/2[633] and 3/2[631] s.p. orbitals
- DSM: β_2 and β_3 determination → correct positions and mutual spacing of the 5/2[633] and 3/2[631] orbitals ⇒ $\beta_2 = 0.240$ and $\beta_3 = 0.115$ ⇒ quasi-spin doublet
- CQOM: parameters fits → ω, b, d_0 (for energy levels); c, p (transition probabilities); K-mixing constant A (energies and transitions)
- BCS: pairing constants tuning → $g_0 = 18.805$, $g_1 = 7.389$ ⇒ $E(3/2^+) \sim 0.07 - 0.4$ keV
- Possible further refinement: ω - oscillator tuning ⇒ $E(3/2^+) \sim 0.0078$ keV → rms deterioration $0.4 - 1.0$ keV

Theoretical and experimental quasi parity-doublet spectrum of ^{229}Th



Theoretical B(E2) and B(M1) transition values for ^{229}Th at different parameter sets

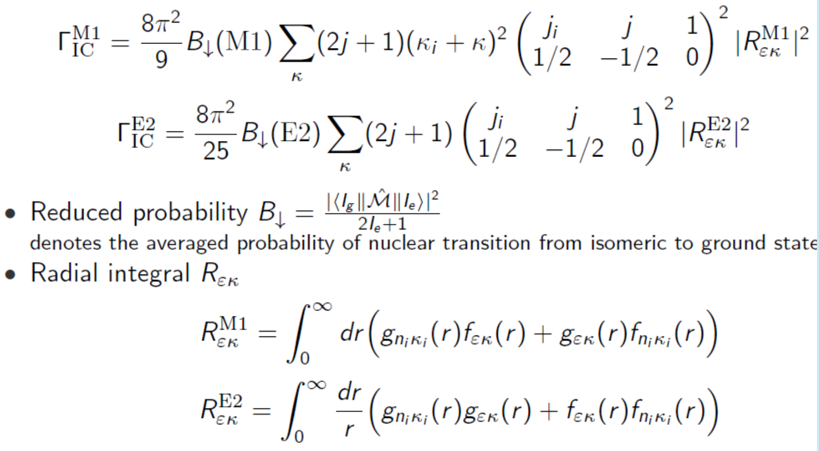
ω	b	d_0	c	p	A	$k_{\text{yr}}^{(-)}$	$k_{\text{ex}}^{(-)}$	rms$_{\text{yr}}$	rms$_{\text{ex}}$	rms$_{\text{tot}}$	$E_{\text{ex}}(\frac{3}{2}^+)$	$B(E2)$	$B(M1)$
0.2039	0.28	18	79	1.0	0.158	2	2	39.9	26.0	34	0.4263	27.04	0.0076
0.2361	0.28	33	89	1.0	0.141	2	2	41.2	26.4	35	0.0078	23.05	0.0061
0.0912	2.39	49	245	1.0	0.152	4	6	37.6	15.8	29	0.3556	25.80	0.0071
0.0635	4.51	45	321	1.0	0.144	6	8	36.4	12.4	28	0.0725	22.86	0.0063
0.0563	7.34	66	473	1.0	0.138	8	10	38.3	11.9	29	10^{-9}	21.31	0.0058

⇒ transition probabilities for the $3/2^+$-isomer decay in ^{229}Th expected in the limits:

$B(E2)$=20–30 W.u.
$B(M1)$=0.006–0.008 W.u.

N. M. and A. Pálffy, Phys. Rev. Lett. **118**, 212501 (2017)
N. M. Bulg. J. Phys. **44**, 434 (2017)

Application to IC rates and lifetimes estimation



$$\Gamma^{\mathrm{M1}}_{\mathrm{IC}} = \frac{8\pi^2}{9} B_\downarrow(\mathrm{M1}) \sum_\kappa (2j+1)(\kappa_i+\kappa)^2 \begin{pmatrix} j_i & j & 1 \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 |R^{\mathrm{M1}}_{\varepsilon\kappa}|^2$$

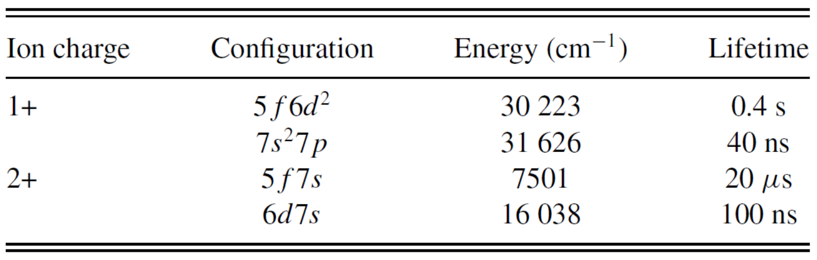
$$\Gamma^{\mathrm{E2}}_{\mathrm{IC}} = \frac{8\pi^2}{25} B_\downarrow(\mathrm{E2}) \sum_\kappa (2j+1) \begin{pmatrix} j_i & j & 1 \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 |R^{\mathrm{E2}}_{\varepsilon\kappa}|^2$$

- Reduced probability $B_\downarrow = \frac{|\langle I_g \| \hat{\mathcal{M}} \| I_e \rangle|^2}{2I_e+1}$
  denotes the averaged probability of nuclear transition from isomeric to ground state
- Radial integral $R_{\varepsilon\kappa}$

$$R^{\mathrm{M1}}_{\varepsilon\kappa} = \int_0^\infty dr \Big(g_{n_i\kappa_i}(r) f_{\varepsilon\kappa}(r) + g_{\varepsilon\kappa}(r) f_{n_i\kappa_i}(r) \Big)$$

$$R^{\mathrm{E2}}_{\varepsilon\kappa} = \int_0^\infty \frac{dr}{r} \Big(g_{n_i\kappa_i}(r) g_{\varepsilon\kappa}(r) + f_{\varepsilon\kappa}(r) f_{n_i\kappa_i}(r) \Big)$$

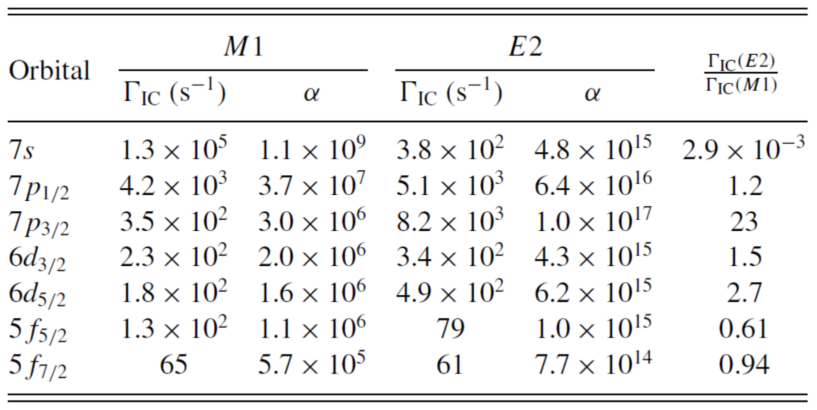
Lifetimes of excited electronic states in $^{229}\mathrm{Th}^+$ calculated through the isomer B(M1) and B(E2) values



Ion charge	Configuration	Energy (cm^{-1})	Lifetime
1+	$5f6d^2$	30 223	0.4 s
	$7s^27p$	31 626	40 ns
2+	$5f7s$	7501	20 μs
	$6d7s$	16 038	100 ns

P. Bilous, G. Kazakov, I. Moore, T. Schumm and A. Pálffy, PRA **95**, 032503 (2017)

Predicted Γ(M1) and Γ(E2) IC rates for electronic states in ^{229}Th calculated through the isomer B(M1) and B(E2) values



Orbital	$M1$		$E2$		$\frac{\Gamma_{\mathrm{IC}}(E2)}{\Gamma_{\mathrm{IC}}(M1)}$
	Γ_{IC} (s^{-1})	α	Γ_{IC} (s^{-1})	α	
$7s$	1.3×10^5	1.1×10^9	3.8×10^2	4.8×10^{15}	2.9×10^{-3}
$7p_{1/2}$	4.2×10^3	3.7×10^7	5.1×10^3	6.4×10^{16}	1.2
$7p_{3/2}$	3.5×10^2	3.0×10^6	8.2×10^3	1.0×10^{17}	23
$6d_{3/2}$	2.3×10^2	2.0×10^6	3.4×10^2	4.3×10^{15}	1.5
$6d_{5/2}$	1.8×10^2	1.6×10^6	4.9×10^2	6.2×10^{15}	2.7
$5f_{5/2}$	1.3×10^2	1.1×10^6	79	1.0×10^{15}	0.61
$5f_{7/2}$	65	5.7×10^5	61	7.7×10^{14}	0.94

P. Bilous, N.M. and A. Pálffy, PRC **97**, 044320 (2018)

$B(M1)$=0.0076 W.u.

$B(E2)$=27 W.u. from the CQOM calculations

Concluding remarks

- Model: CQOM+DSM+BCS with Coriolis mixing - description of K-suppressed E/M transitions at axial symmetry
- Application: test of nuclear-shape effects at the border of atomic energy scale – 7.8 eV ^{229m}Th isomer → effect of quadrupole-octupole-shape driven quasi parity-doublet structure with 5/2[633]-3/2[631] quasi-spin symmetry
- $3/2^+$ state interpretation: a bandhead of an excited quasi parity-doublet, built on 3/2[631] q.p. state coupled to a collective quadrupole-octupole vibration mode and rotation motion - remarkably fine interplay between all these modes!
- Suggestion: Shape and symmetry driven E/M properties of nuclei manifest in unexpectedly wide energy ranges
- Questions: To what extent nuclear shape dynamics can govern effects in the atomic energy scale? What about ^{235m}U? Could we expect similar effects in other nuclei?