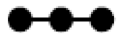
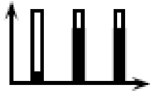
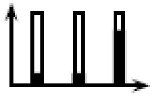
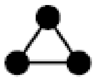
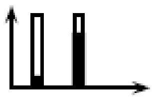
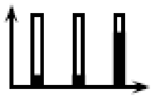
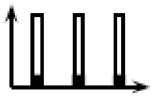
How to determine the shape of nuclear molecules with polarized γ-rays :: EFB24 – 05/09/2019

name	shape	group	Γ_{vib}	Patterns
linear =		$\mathcal{D}_{\infty h}$	$A_{1g} + A_{1u} + E_{1u}$	
linear ≠		$\mathcal{C}_{\infty\nu}$	$2A_1 + E_1$	
equilateral		$\mathcal{D}_{3h}$	$A_1' + E'$	
isosceles		$\mathcal{C}_{2\nu}$	$2A_1 + B_1$	
scalene		$\mathcal{C}_s$	$3A'$	

Lorenzo Fortunato
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Italy

Outline of the presentation

- Polarized gamma beams: scenario for future measurements
- Molecular nuclear structure and discrete symmetries
- Electromagnetic probes
- Polarizability and active modes
- Depolarization ratio and character identification
- The case of 12C and more exotic structures
- Transition densities

PHYSICAL REVIEW C **99**, 031302(R) (2019)

Rapid Communications | Editors' Suggestion

Establishing the geometry of α clusters in ^{12}C through patterns of polarized γ rays

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(Received 13 December 2018; published 11 March 2019)

Polarized gamma-ray facilites around the globe:

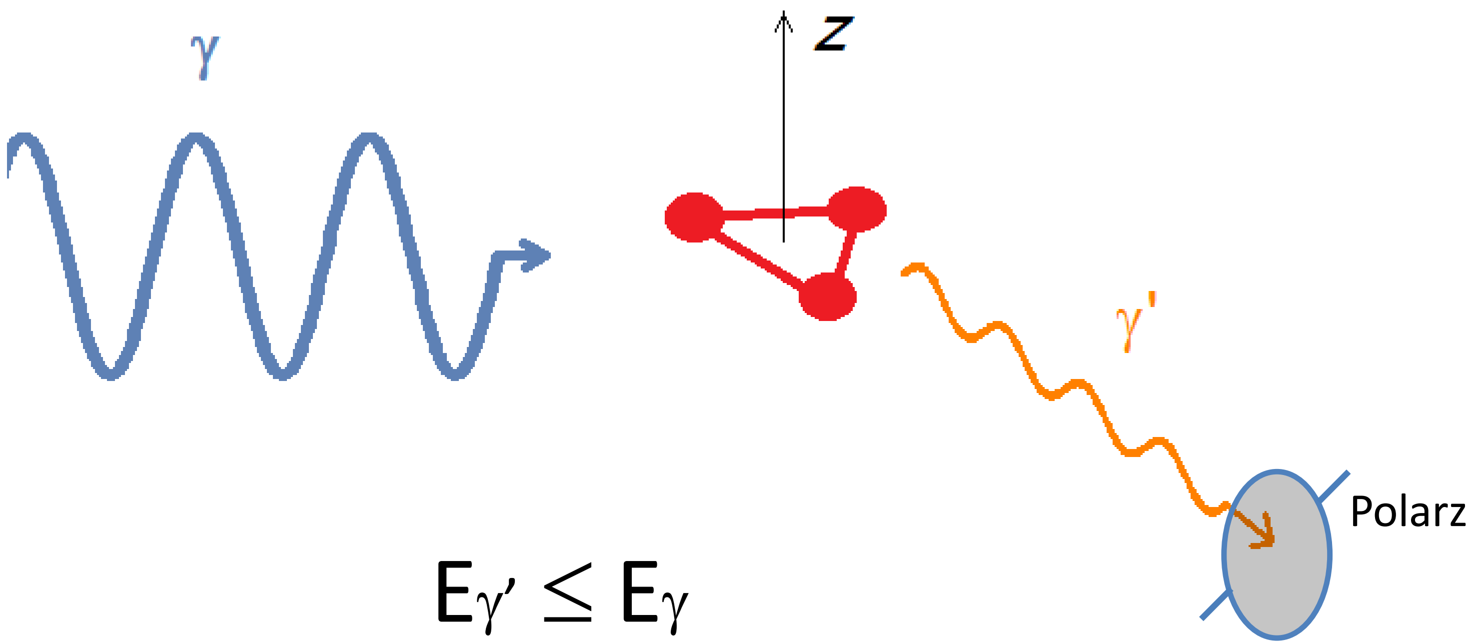
- Mainz Microtron MAMI (Continuous Wave, beam polarization 80%, En. resol. 0.1 MeV, but energy too high 50-800 MeV)
- Triangle University Higs facility (FEL type, quasi CW operation, 2-60 MeV, flus 10^8-10^9 phot./s)
- ELI-NP in Romania (0-20 MeV, high flux, high resolution, 100% polarization)
- LEPS – Japan (very high energy)
- NewSubaru
- …

eli Extreme Light Infrastructure
Nuclear Physics (ELI-NP)

Gamma beam parameter	Value
Energy [MeV]	0.2 – 19.5
Spectral density [ph/s/eV]	$0.8 - 4{\cdot}10^{4}$
Bandwidth rms [%]	≤ 0.5
#Photons/shot within FWHM bdw.	$\leq 2.6{\cdot}10^{5}$
#Photons/s within FWHM bdw.	$\leq 8.3{\cdot}10^{8}$
Source rms size [μm]	10 – 30
Source rms divergence [μrad]	25 – 200
Peak brilliance [N_{ph}/s·mm^2·mrad^2·0.1%bdw]	$10^{20} - 10^{23}$
Pulse length rms [ps]	0.7 – 1.5
Linear polarization [%]	> 99
Macro repetition rate [Hz]	100
Number of pulses/macropulse	32
Pulse–to–pulse separation [ps]	16

With the advent of the new facility in Romania, beams of high brilliance, focused, polarized gamma rays produced with Inverse Compton Scattering will become available with energies ranging from 0.2-20 MeV

One can shoot linearly polarized gamma rays (Electric field oscillating in a given direction constant in time) of appropriate energy (tuned to match the resonances of interest) and observe the outcoming gammas of the same or different energies with a polarizer/analyzer.



$$E_{\gamma'} \leq E_{\gamma}$$

If the nucleus has a definite geometrical symmetry (i.e. if there is an underlying discrete group structure), very strict selection rules apply.

Experimentally the polarization can be measured with another inverse Compton scattering

Depolarization ratio

One can measure the so-called depolarization ratio between intensities, by turning the analyzer/polarizer of 90 degrees, i.e.:

$$\rho = \frac{I_\perp}{I_\parallel}$$

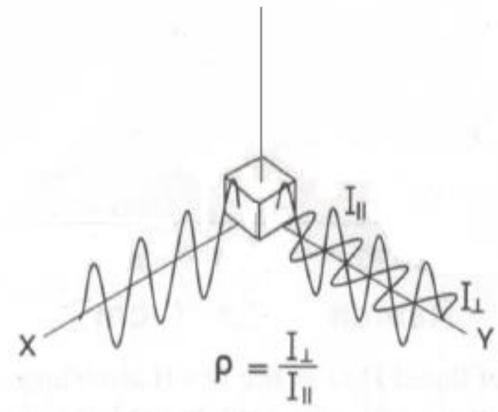


Figure 8.6. Parallel and perpendicular Raman scattering.

as a tool to determine which modes are totally symmetric modes. In fact from the theory of Raman scattering

$0 \leq \rho \leq \frac{3}{4}$ for polarized bands (symmetric modes)

$\rho = \frac{3}{4}$ for depolarized bands (non-symmetric modes)

even with a randomly oriented sample.

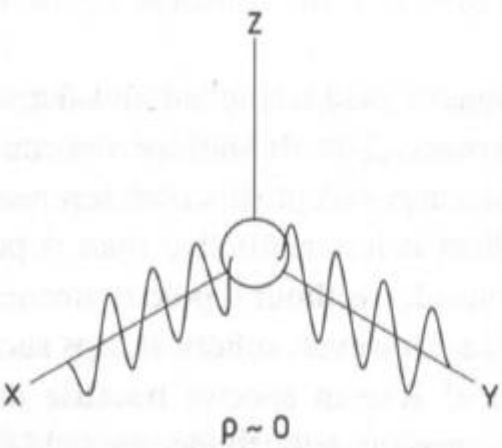


Figure 8.8. Polarized light scattering by a sphere.

Figures from book by P.Bernath

Depolarization ratio : a chemical example CCl_4

This kind of measuments of $\rho = \frac{I_\perp}{I_\parallel}$ are absolutely standard in optical spectroscopy (where polarizers and analyzers are easy to do and handle).

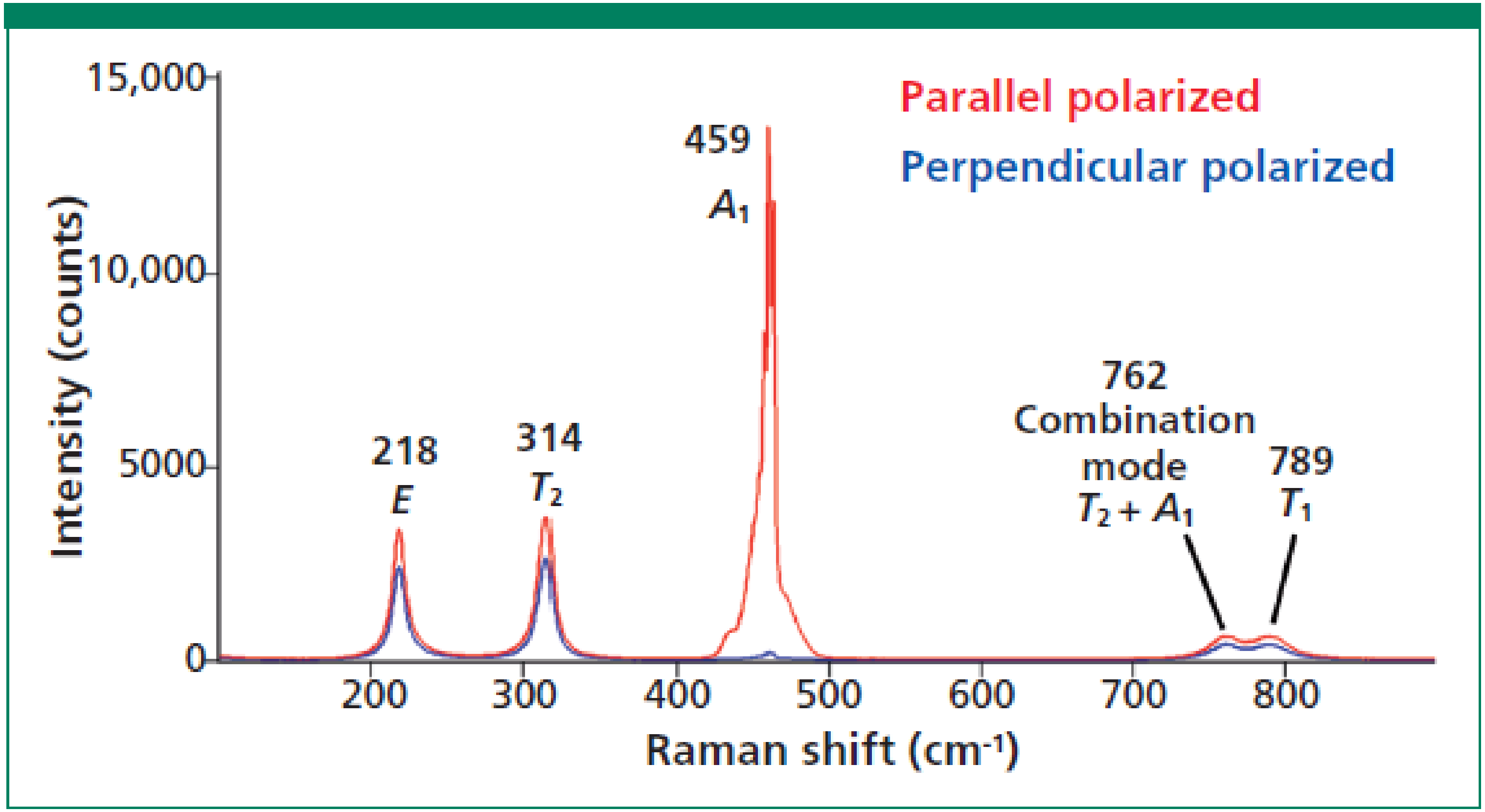
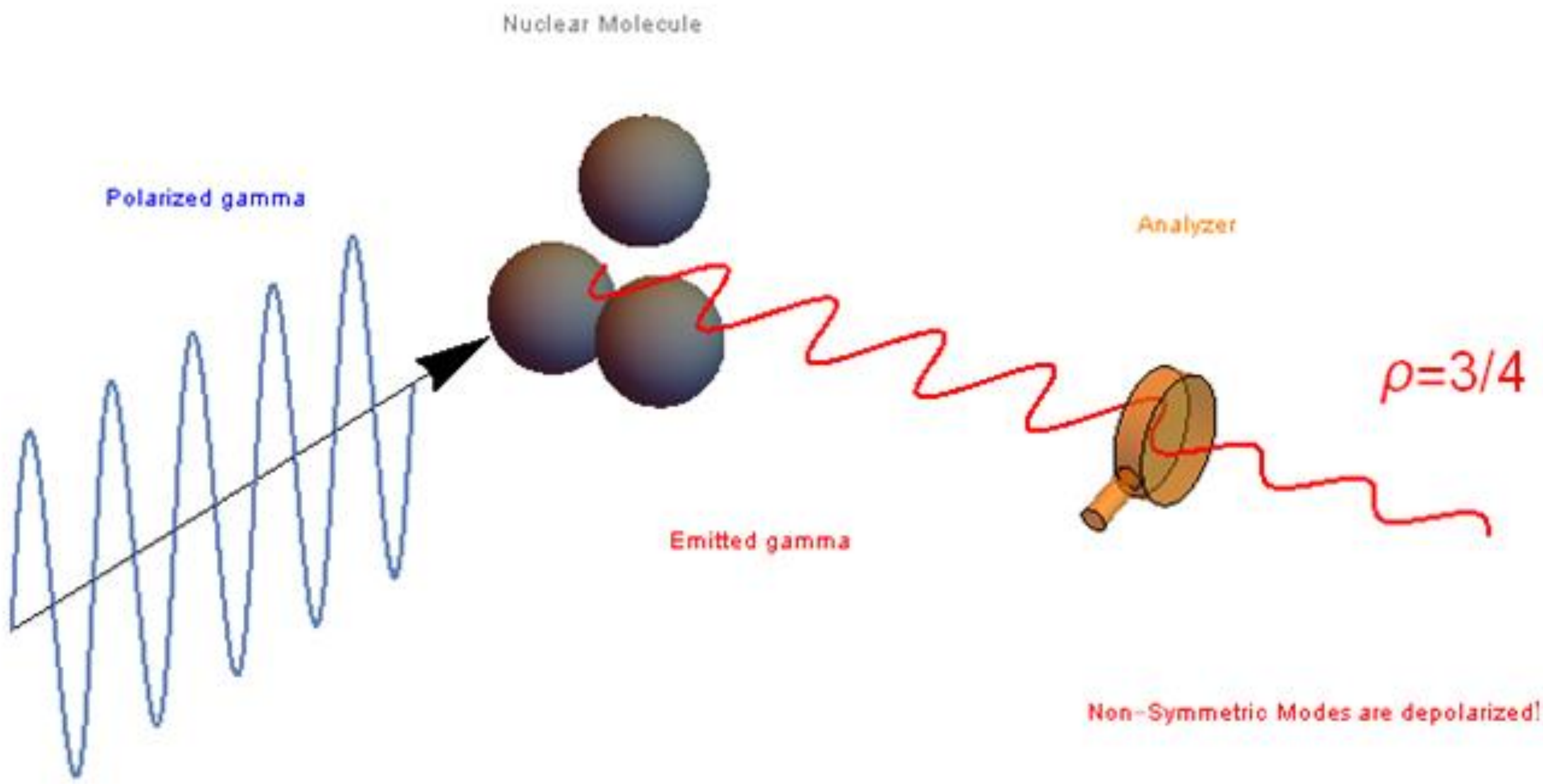


Figure 2: Polarized Raman spectra of CCl_4.

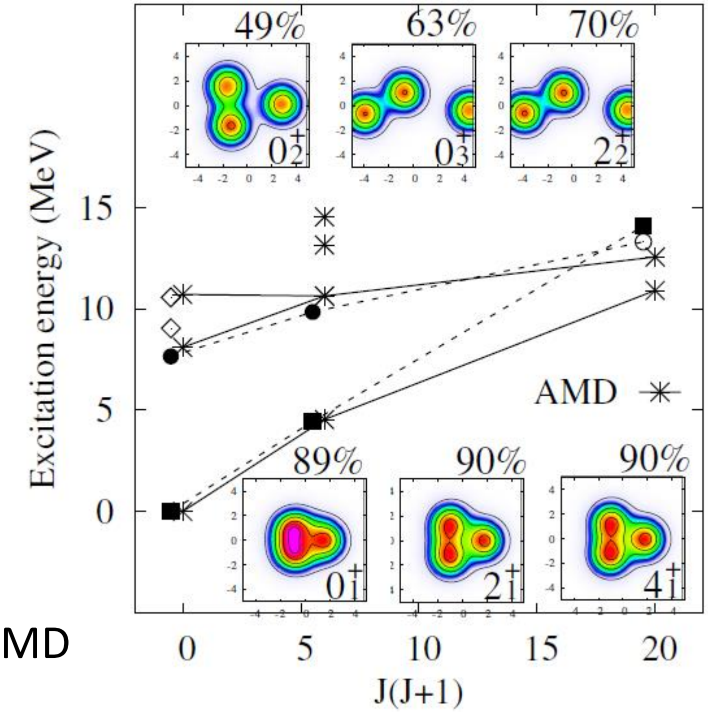
Figure from D.Tuschel – Spectroscopy (2014)

Depolarization ratio

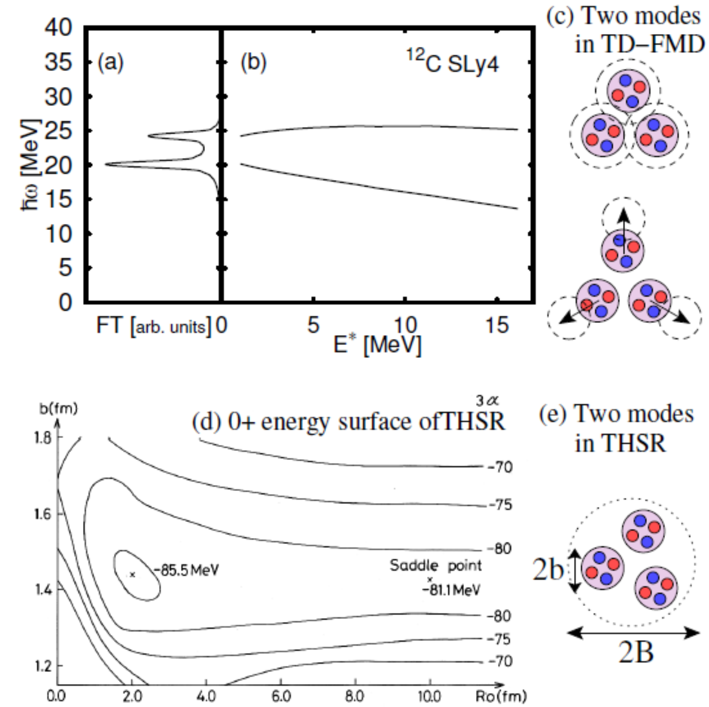


Panoply of different models …

(Too) many models have been proposed for 12C where the triangle is not equilateral, isosceles, scalene or even a linear chain (Morinaga). Therefore I have set forth to determine all possible outcomes and the patterns that can be predicted are intended as a guidance as to which configuration is right and **the tell-tale method is clearly through measurements of the depolarization ratio in Raman-like experiments of nuclear fluorescence** that will be feasible at ELI-NP or in other labs where gamma-rays are available.



AMD



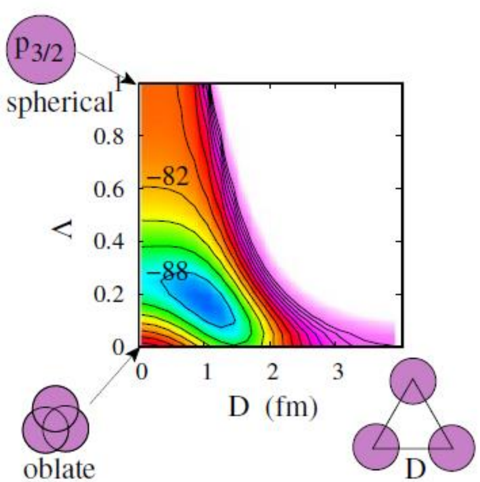
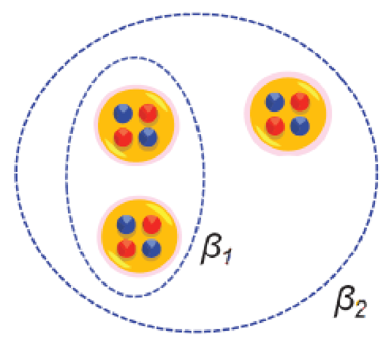


FIG. 10 (Color online) 0^+-projected energy surface on the Λ-D plane for ^{12}C calculated by the AQCM. The interaction and width parameters are same as those in Ref. (Suhara *et al.*, 2013).



Figures from: Freer et al. (2018) Microscopic clustering in Light Nuclei

Algebraic cluster model for 3 alphas

Bijker and Iachello have clearly demonstrated the succesfull application of the ACM, or algebraic cluster model, to the vibrational-rotational spectrum of alpha-conjugate nuclei like 12C and 16O.

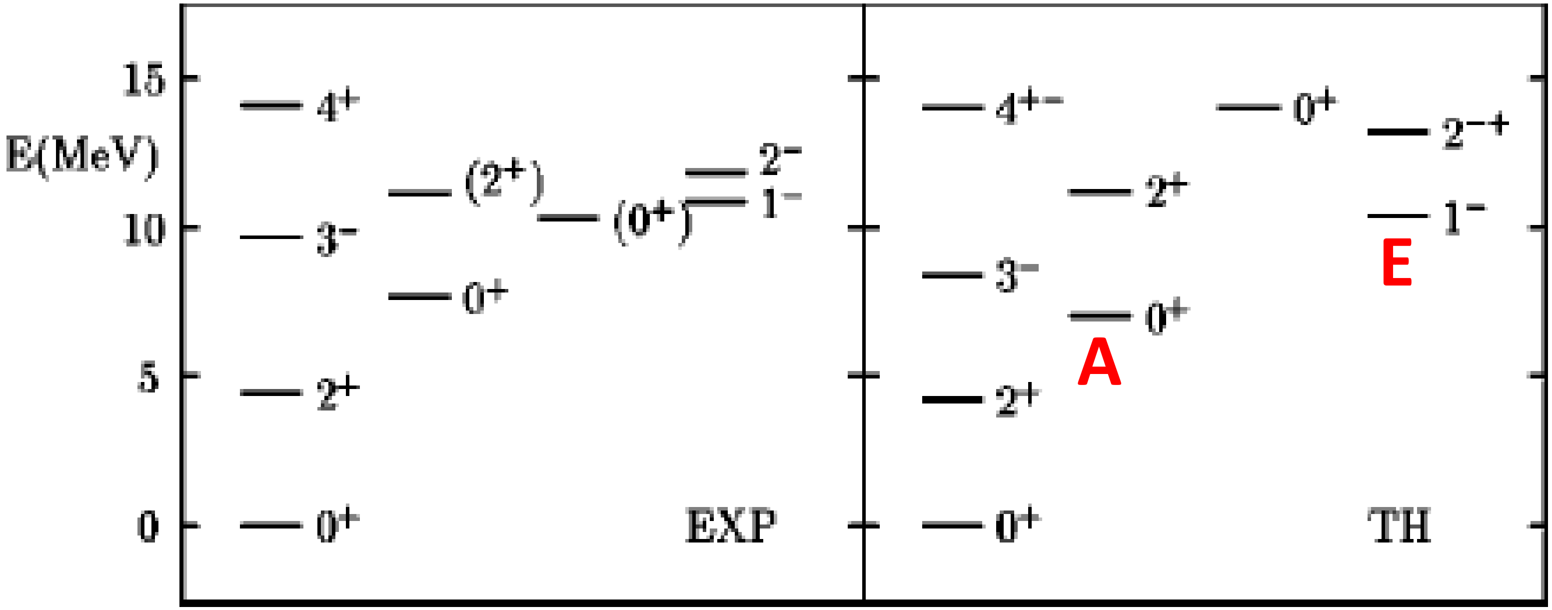
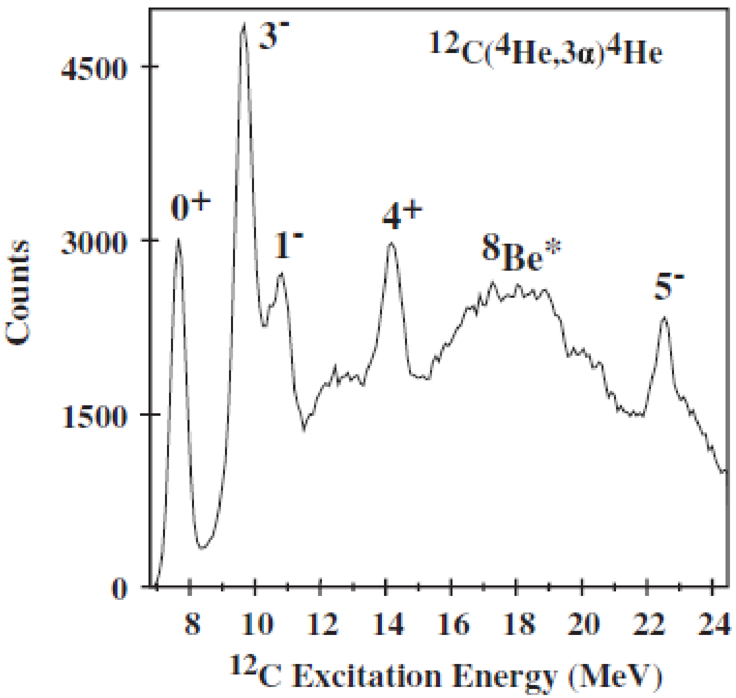


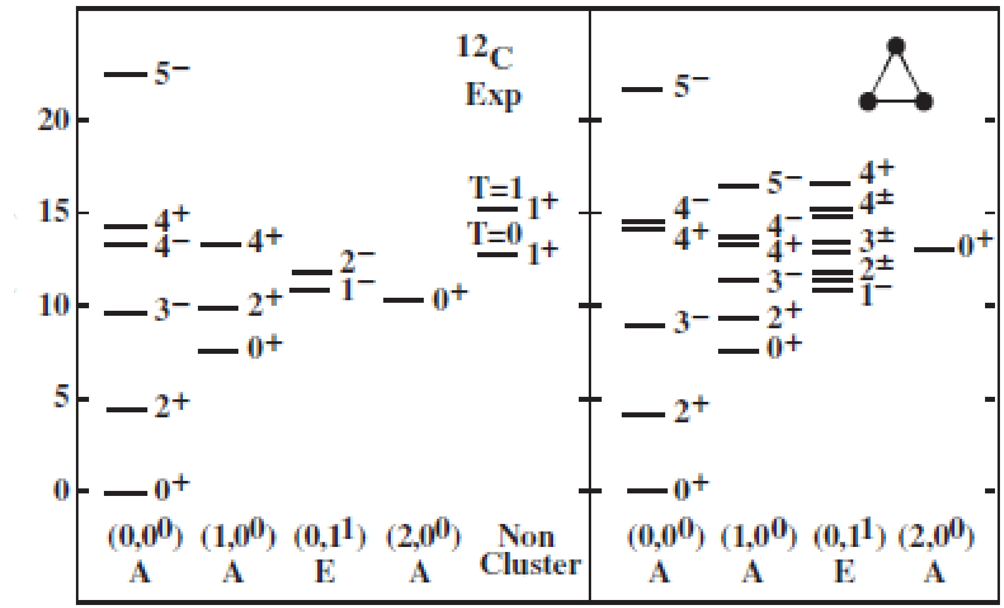
FIG. 2. Comparison between the low-lying experimental spectrum of ^{12}C [12] and that calculated using Eq. (6) with $A=7.0$, $B=9.0$, $C=0.7$, and $D=0.0$ MeV. States with uncertain spin-parity assignment are in parentheses.

PRL 113, 012502 (2014) PHYSICAL REVIEW LETTERS week ending 4 JULY 2014

Evidence for Triangular $\mathcal{D}_{3h}$ Symmetry in ^{12}C

D. J. Marín-Lámbarri,[1] R. Bijker,[2] M. Freer,[1] M. Gai,[3,4] Tz. Kokalova,[1] D. J. Parker,[1] and C. Wheldon[1]





This lovely paper confirms the assignation of the 5- state at 22.4(2) MeV to the g.s. band of an **equilater triangular structure.**

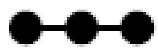
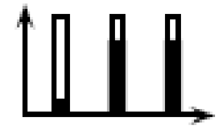
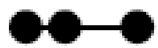
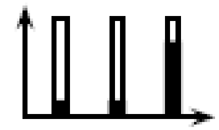
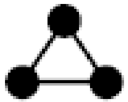
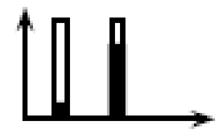
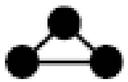
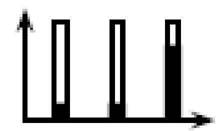
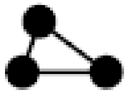
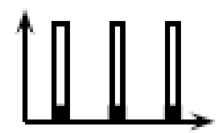
Note the uncommon spin-parity of bands (the doublet 4+/ 4- has a natural explanation in terms of D3h symmetry!).

Different geometric arrangements of equilibrium points → Discrete symmetry group → Precise selection rules

Work plan:

- Decide arrangement of N particles
- This means 3N-6 d.o.f (or 3N-5 d.o.f. for linear arrangement)
- Identify the underlying discrete group structure
- Find the character under transformations of the group Γ_{3N}
- Subtract translations and rotations to single out character of vibrational modes Γ_{vib}
- Identify patterns of totally symmetric modes
- Check models against measures of intensities $\rightarrow$ Eureka !!

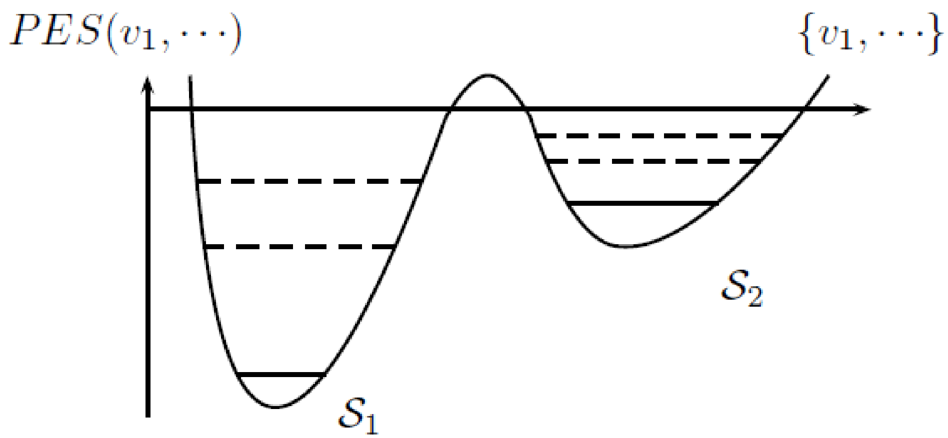
Tables in PRC 99 (2019) paper: 3 equal clusters

name	shape	group	Γ_{vib}	Patterns
linear =		$\mathcal{D}_{\infty h}$	$A_{1g} + A_{1u} + E_{1u}$	
linear ≠		$\mathcal{C}_{\infty \nu}$	$2A_1 + E_1$	
equilateral		$\mathcal{D}_{3h}$	$A_1' + E'$	
isosceles		$\mathcal{C}_{2\nu}$	$2A_1 + B_1$	
scalene		$\mathcal{C}_s$	$3A'$	

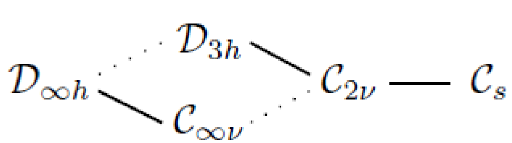
The number of totally symmetric peaks over total is different in each case, therefore one can disentagle the various possibilities

Tables in PRC 99 (2019) paper

There might be more than just one configuration! The picture complicates a little, but not too much ! One can invoke the concept of descent in symmetry ans still aplly some of the rules.



Group chains



$\mathcal{D}_{\infty h}$	$A_{1g}+$	$A_{1u}+$	E_{1u}
$\mathcal{C}_{\infty v}$	A_1+	A_1+	E_1
$\mathcal{C}_{2v}$	A_1+	A_1+	$B_1 + B_2$
$\mathcal{C}_s$	$A'+$	$A'+$	A'

$\mathcal{D}_{\infty h}$	$A_{1g}+$	$A_{1u}+$	E_{1u}
$\mathcal{D}_{3h}$	$A_1'+$	$A_2''+$	E'
$\mathcal{C}_{2v}$	A_1+		$A_1 + B_1$
$\mathcal{C}_s$	$A'+$		$A' + A'$

FIG. 4. Descent in symmetry restricted to representations of the groups that are relevant to all possible configurations of three identical particles.

Tetrahedral shape in 16 Oxygen

Bijker, Iachello
PRL 112, 152501 (2014)

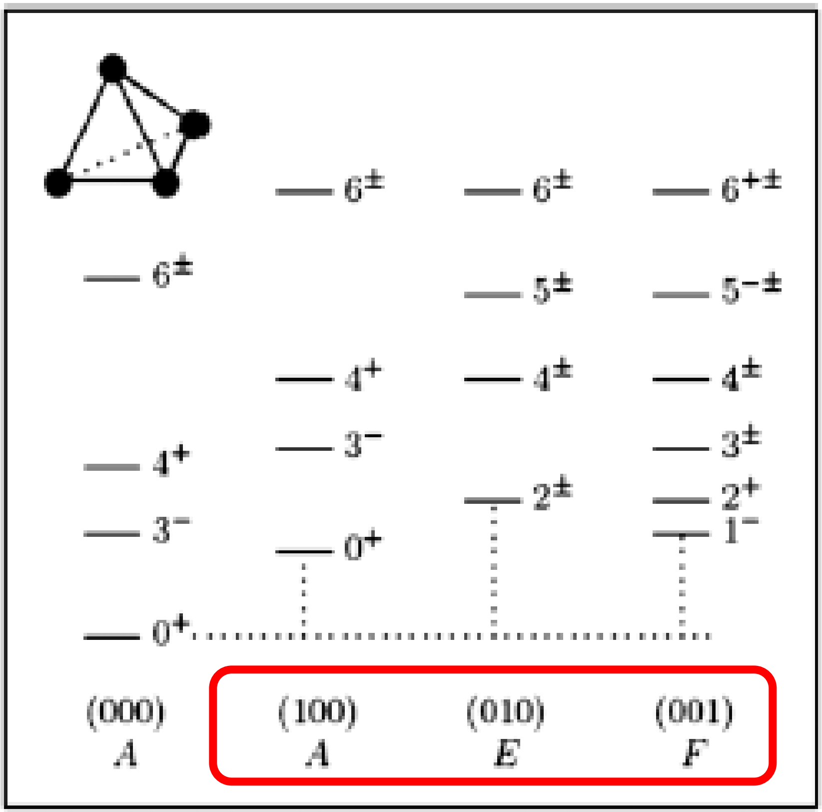
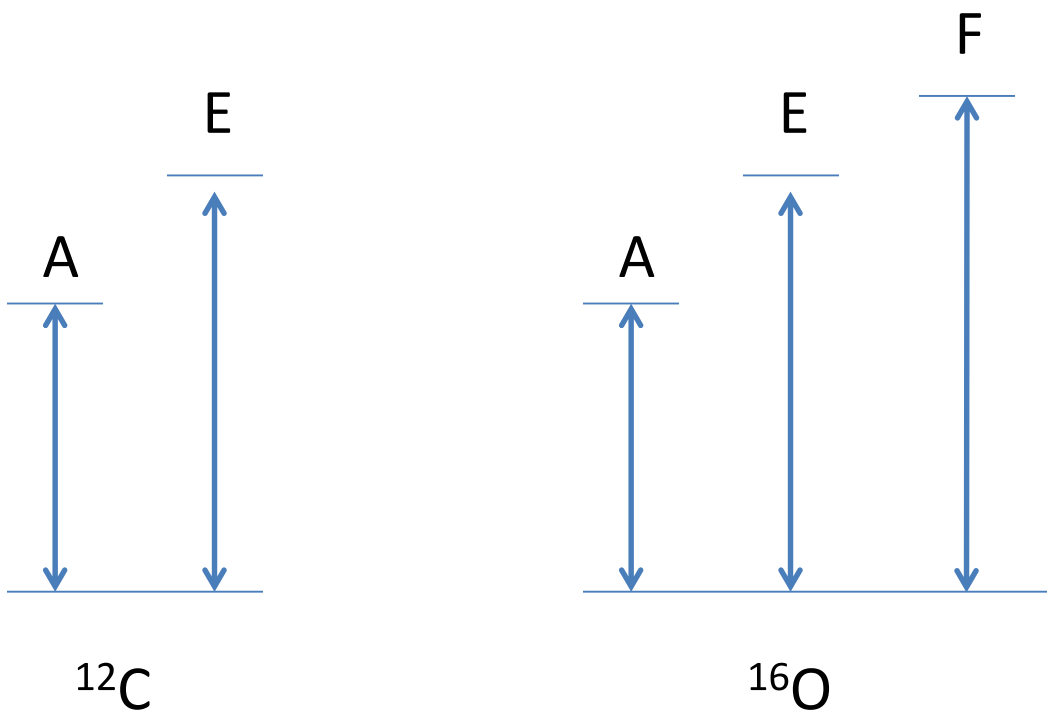
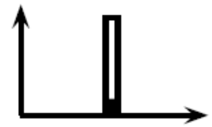
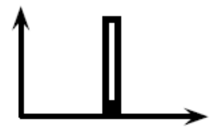


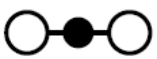
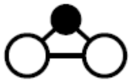
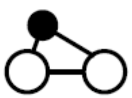
FIG. 1. Schematic spectrum of a spherical top with tetrahedral symmetry and $\omega_1 = \omega_2 = \omega_3$. The rotational bands are labeled by (v_1, v_2, v_3) (bottom). All states are symmetric under S_4.

They use a somewhat simplified notation based on the permutation (sub)groups S_3 and S_4 of the full discrete groups D_{3h} and T_d respectively , but the essence is the same.

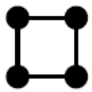


Tables for 2 clusters and for 3 clusters of type AAB

name	shape	group	Γ_{vib}	Patterns
linear AA		$\mathcal{D}_{\infty h}$	A_{1g}	
linear AB		$\mathcal{C}_{\infty \nu}$	A_1	

name	shape	group	Γ_{vib}	Patterns
linear ABA		$\mathcal{D}_{\infty h}$	$A_{1g} + A_{1u} + E_{1u}$	
linear AAB		$\mathcal{C}_{\infty \nu}$	$2A_1 + E_1$	
isosceles AAB		$\mathcal{C}_{2\nu}$	$2A_1 + B_1$	
scalene AAB		$\mathcal{C}_s$	$3A'$	

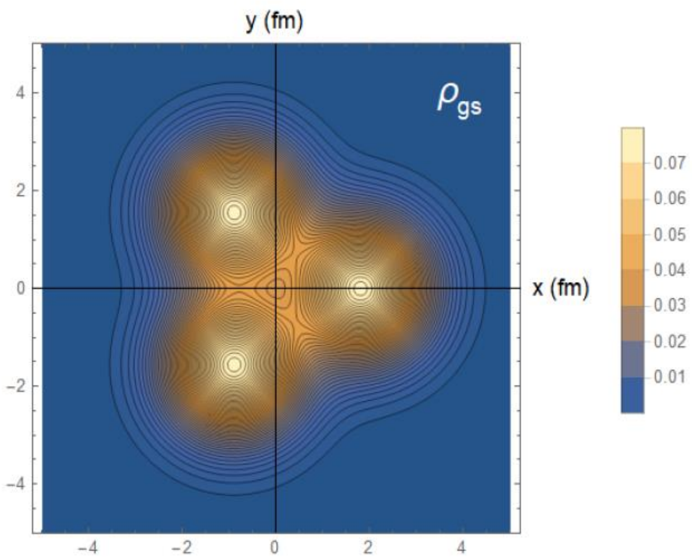
Tables for 4clusters, only some have been worked out

name	shape	group	Γ_{vib}	Patterns
linear aaa		$\mathcal{D}_{\infty h}$	$2A_{1g} + E_{1g} + E_{4g} + A_{1u} + E_{1u}$	2/6
linear aba		$\mathcal{D}_{\infty h}$	$2A_{1g} + E_{1g} + A_{1u} + E_{1u}$	2/5
square a^4b^2		$\mathcal{D}_{4h}$	$A_{1g} + B_{1g} + B_{2g} + B_{2u} + E_u$	1/5
kite a^4bc		$\mathcal{D}_{2h}$	$2A_g + B_{1g} + B_{1u} + B_{2u} + B_{3u}$	2/6
centered eq. triangle a^3b^3		$\mathcal{D}_{3h}$	$A'_1 + 2E' + A''_2$	1/4
rectangle $a^2b^2c^2$		$\mathcal{D}_{2h}$	$2A_g + B_{1g} + A_u + B_{2u} + B_{3u}$	2/6
tetrahedron a^6		$\mathcal{T}_d$	$A_1 + E + T_2$	1/3
uneq. tetrah. a^3b^3		$\mathcal{C}_{3v}$	$2A_1 + 2E$	2/4
wedge a^4b^2		$\mathcal{D}_{2d}$	$2A_1 + B_1 + B_2 + E$	2/5
2 triangles at 90^o a^5b		$\mathcal{C}_{2v}$	$3A_1 + A_2 + B_1 + B_2$	3/6

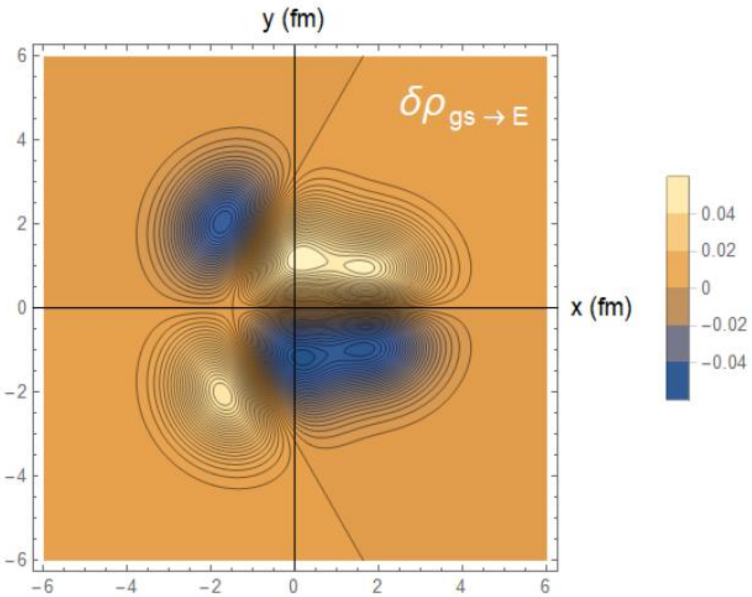
- One might gather information on polarization due to alpha particles' substructures

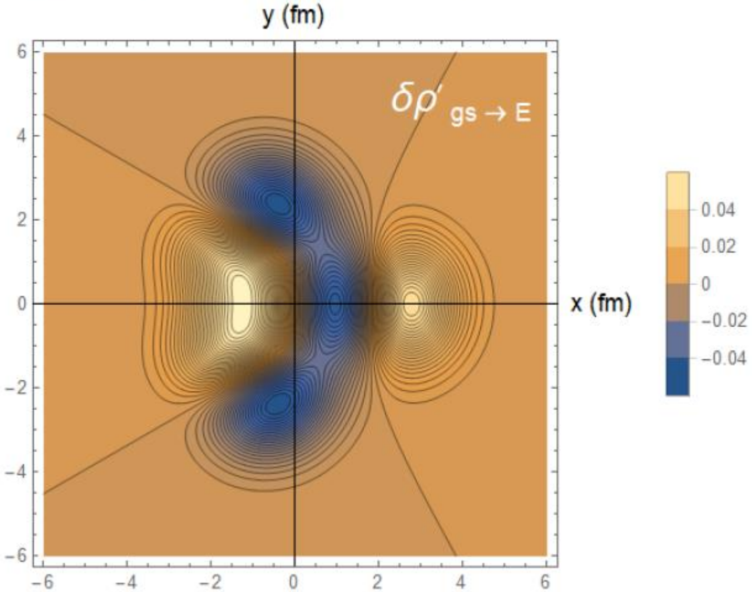
Recent work on transition densities in 12C

In collaboration with A. Vitturi, E. Lanza and J. Casal



Ground state





Summary

- ✓ I have suggested to use the **highly polarized monochromatic gamma rays** that will be available at ELI-NP as a **tool to study the molecular vibrations of clusterized nuclei**, taking as a definite example the 12C nucleus as composed of 3 α particles. Extended to 2, 3 unequal and 4 clusters.

- ✓ I believe that, if a **measure of depolarization ratio** could be done in a sort of Raman nuclear fluorescence experiment, this would yield **precise patterns of vibrational spectra**, that will **correlate directly** with a given **geometric configuration** possessing a **discrete point-group symmetry**.

- ✓ I have shown some preliminary transition densities for 12C in a molecular model.

1222·2022 800 ANNI
Università degli Studi di Padova
Dipartimento di Fisica e Astronomia Galileo Galilei
INFN Istituto Nazionale di Fisica Nucleare

A few points for discussion

- if the g.s. rotational band contains the same multipolarity that one is trying to excite in the vibrational bands, this is also to be included in the above patterns.

- in principle the degree of polarization might be close to 3/4 also for polarized (A) bands, therefore it might become hard to distinguish between them

- non-cluster degrees of freedom might come into play at a certain energy, thus blurring the picture

- in nuclei with a cluster structure including *t* or *h* clusters, the interplay with single-particle orbits around a molecular center might also be very relevant

- I guess a BEC gas would show no geometric arrangments (no equilibirum points) and would behave as an L=0 state (a sphere), thus offering only 1 such bands of A type (polarized).

A word of caution

DISCLAIMER:

- It is perfectly clear to us that molecular models of nuclei are FUNDAMENTALLY DIFFERENT from molecular physics, where the Born-Oppenheimer approximation is valid and one can think of nuclear motion as a small vibration, happening only close to the minimum of a very deep potential energy surface (in molecular energy scales).

- Nuclei have large kinetic energy <T>, comparable to the potential energy <V> and the zero point motion inside the P.E.S. is a large fraction of the well depth, therefore there are LARGE FLUCTUATIONS around the equilibrium points and we SHOULD NOT EXPECT that the vibrational levels are deeply lying in the potential well, at most they can be weakly bound states, close to threshold, or more probably resonances in the continuum!

- Dispite this, it is instructive to look at
    1. the normal modes, i.e. the «best» internal coordinates
    2. symmetry-adapted vibrational orbitals
    3. the energy scale and structure of the vibrational levels

Table II: The Mulliken symbols used to describe the symmetry species of point groups including their meaning with respect to molecular symmetry

Mulliken Symbols of Symmetry Species (Column 1 In Character Table)	Meaning
A	Symmetric with respect to principal axis of symmetry
B	Antisymmetric with respect to principal axis of symmetry
E	Doubly degenerate, two-dimensional irreducible representation
T	Triply degenerate, three-dimensional irreducible representation
g	Symmetric with respect to a center of symmetry
u	Antisymmetric with respect to a center of symmetry
1 (subscript)	Symmetric with respect to a C_2 axis that is perpendicular to the principal axis. Where there is no such axis the subscript indicates that reflection in a $_v$ plane of symmetry is symmetric.
2 (subscript)	Antisymmetric with respect to a C_2 axis that is perpendicular to the principal axis. Where there is no such axis the subscript indicates that reflection in a $_v$ plane of symmetry is antisymmetric.
′ (prime)	Symmetric with respect to reflection in a horizontal plane of symmetry
″ (double prime)	Antisymmetric with respect to reflection in a horizontal plane of symmetry

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