5.08.18 class 29: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

From CH_4 to SF_6 to C_{60} : a study in spectacular spectral contrasts

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AMOP reference links *(Updated list given on **2nd** and 3rd pages of each class presentation)*

Web Resources - front page | Quantum Theory for the Computer Age | 2014 AMOP

UAF Physics UTube channel | Principles of Symmetry, Dynamics, and Spectroscopy | 2017 Group Theory for QM

Classical Mechanics with a Bang! | 2018 AMOP

Modern Physics and its Classical Foundations

Representaions Of Multidimensional Symmetries In Networks - harter-jmp-1973

Alternative Basis for the Theory of Complex Spectra

- Alternative_Basis_for_the_Theory_of_Complex_Spectra_I_-_harter-pra-1973
- Alternative_Basis_for_the_Theory_of_Complex_Spectra_II_-_harter-patterson-pra-1976
- Alternative_Basis_for_the_Theory_of_Complex_Spectra_III_-_patterson-harter-pra-1977

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978

Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979

Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984

Galloping waves and their relativistic properties - ajp-1985-Harter

Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 (Alt Scan)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

- I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)
- II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)

Rotation–vibration spectra of icosahedral molecules.

- I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989 (Alt.)
- II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989 (Alt scan)
- III) Half-integral angular momentum - harter-reimer-jcp-1991

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)

Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)

Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996

Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)

Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001

Molecular Symmetry and Dynamics - Ch32-Springer Handbooks of Atomic, Molecular, and Optical Physics - Harter-2006

Resonance and Revivals

- I) QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 (Talk) OSU knowledge Bank
- II) Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talks)
- III) Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - (2013-Li-Diss)

Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talk)

Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013

Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013

QTCA Unit 10 Ch 30 - 2013

AMOP Ch 0 Space-Time Symmetry - 2019

**In development - a web based A.M.O.P. oriented reference page, with thumbnail/previews, greater control over the information display, and eventually full on* Apache-SOLR *Index and search for* nuanced, whole-site content/metadata level *searching.*

AMOP reference links *(Updated list given on 2nd and **3rd** pages of each class presentation)*

Int.J.Mol.Sci, 14, 714(2013) p.755-774, *QTCA Unit 8 Ch. 23-25*, *QTCA Unit 9 Ch. 26*, *PSDS Ch. 5*, *PSDS Ch. 7*

Intro spin ½ coupling
Unit 8 Ch. 24 p3

H atom hyperfine-B-level crossing
Unit 8 Ch. 24 p15

Hyperf. theory Ch. 24 p48.

Hyperf. theory Ch. 24 p48.
Deeper theory ends p53

Intro 2p3p coupling
Unit 8 Ch. 24 p17.

Intro LS-jj coupling
Unit 8 Ch. 24 p22.

CG coupling derived (start)
Unit 8 Ch. 24 p39.

CG coupling derived (formula)
Unit 8 Ch. 24 p44.

Lande' g-factor
Unit 8 Ch. 24 p26.

Irrep Tensor building
Unit 8 Ch. 25 p5.

Irrep Tensor Tables
Unit 8 Ch. 25 p12.

Wigner-Eckart tensor Theorem.
Unit 8 Ch. 25 p17.

Tensors Applied to d,f-levels.
Unit 8 Ch. 25 p21.

Tensors Applied to high J levels.
Unit 8 Ch. 25 p63.

Intro 3-particle coupling.
Unit 8 Ch. 25 p28.

Intro 3,4-particle Young Tableaus
GrpThLect29 p42.

Young Tableau Magic Formulae
GrpThLect29 p46-48.

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Predrag Cvitanovic's: Birdtrack Notation, Calculations, and Simplification

Group Theory - PUP_Lucy_Day_-_Diagrammatic_notation_-_Ch4-2008

Group Theory - Birdtracks_Lies_and_Exceptional_Groups_-_Cvitanovic-2011

Simplification_Rules_for_Birdtrack_Operators_-_Alcock-Zeilinger-Weigert-zeilinger-jmp-2017

Birdtracks for SU(N) - 2017-Keppeler

Chaos_Classical_and_Quantum_-_2018-Cvitanovic-ChaosBook

*

Frank Rioux's: UMA method of vibrational induction

Quantum_Mechanics_Group_Theory_and_C60_-_Frank_Rioux_-_Department_of_Chemistry_Saint_Johns_U

Symmetry_Analysis_for_H20-_H20GrpTheory-_Rioux

Quantum_Mechanics-Group_Theory_and_C60_-_JChemEd-Rioux-1994

Group_Theory_Problems-_Rioux-_SymmetryProblemsX

Comment_on_the_Vibrational_Analysis_for_C60_and_Other_Fullerenes_Rioux-RSP

*

Supplemental AMOP Techniques & Experiment

Many Correlation Tables are Molien Sequences - Klee (Draft 2016)

High-resolution_spectroscopy_and_global_analysis_of_CF4_rovibrational_bands_to_model_its_atmospheric_absorption-_carlos-Boudon-jqsrt-2017

Symmetry and Chirality - Continuous_Measures_-_Avnir

*

Special Topics & Colloquial References

r-process_nucleosynthesis_from_matter_ejected_in_binary_neutron_star_mergers-PhysRevD-Bovard-2017

*

Contributions to the International Symposia on Molecular Spectroscopy

Columbus 2002

Columbus 2004

Columbus 2006

Columbus 2007(II)

*

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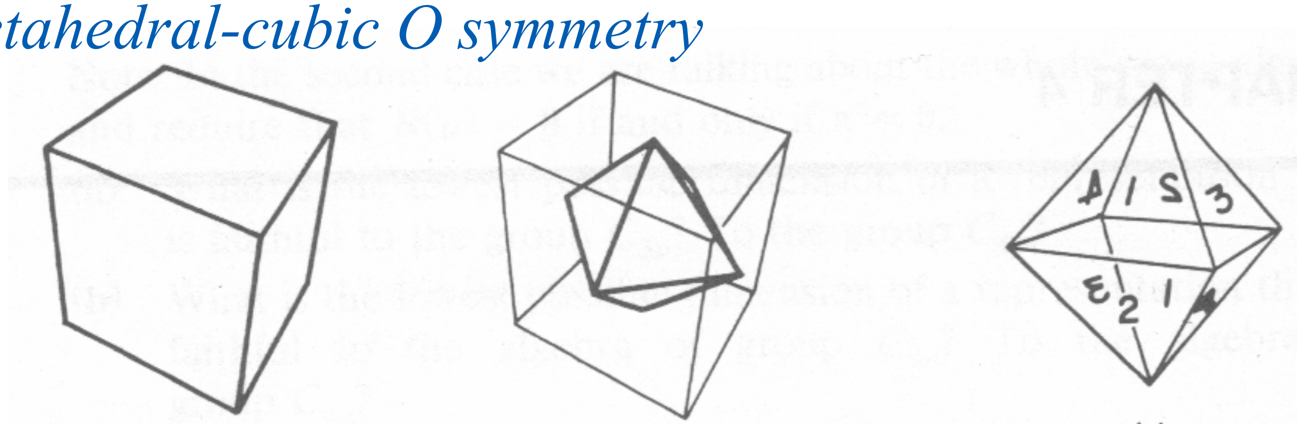
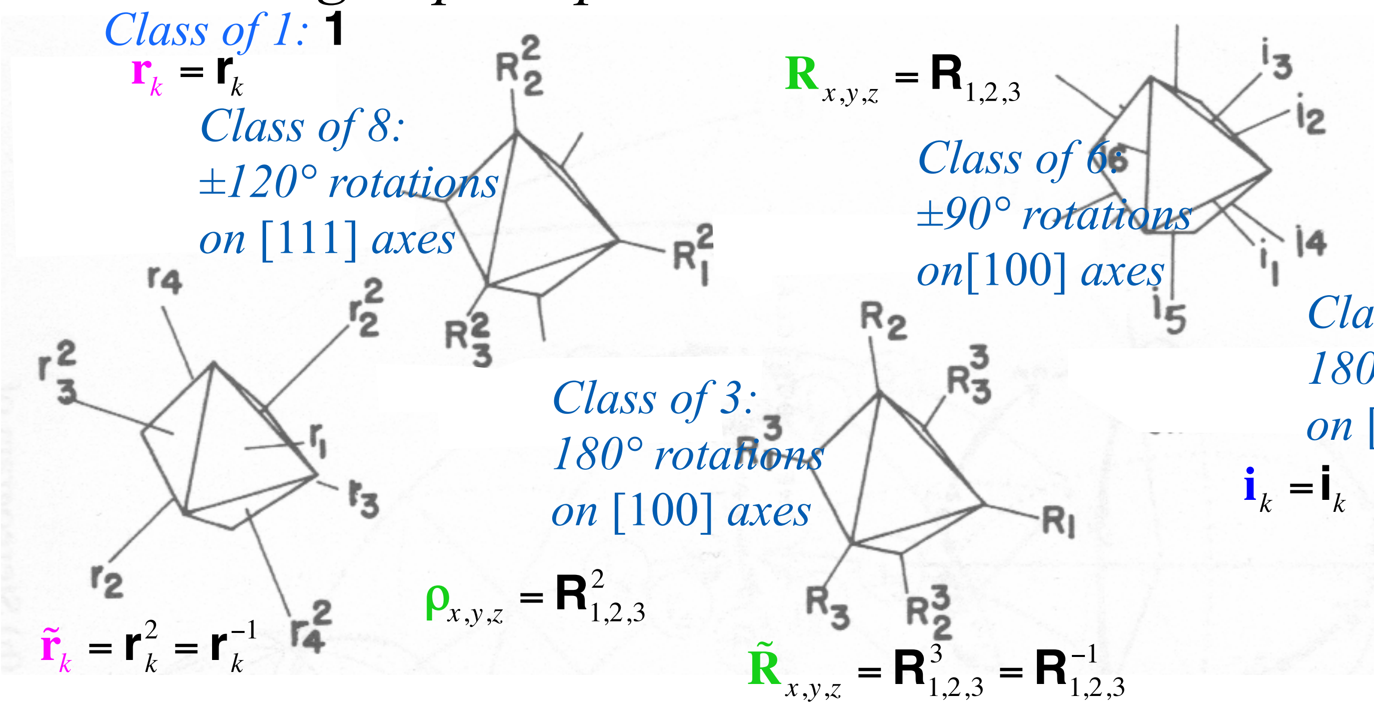
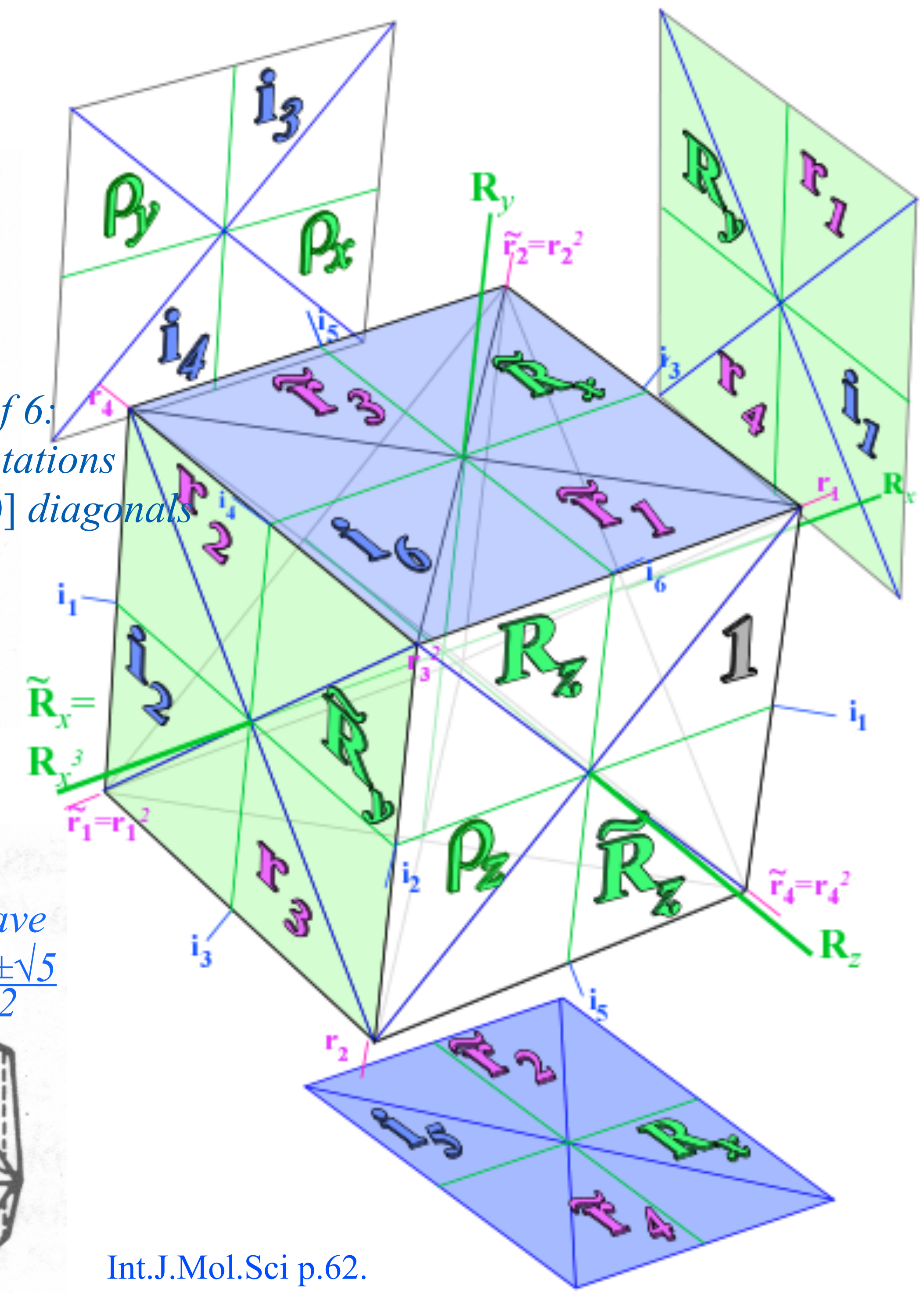
Octahedral-cubic O symmetry



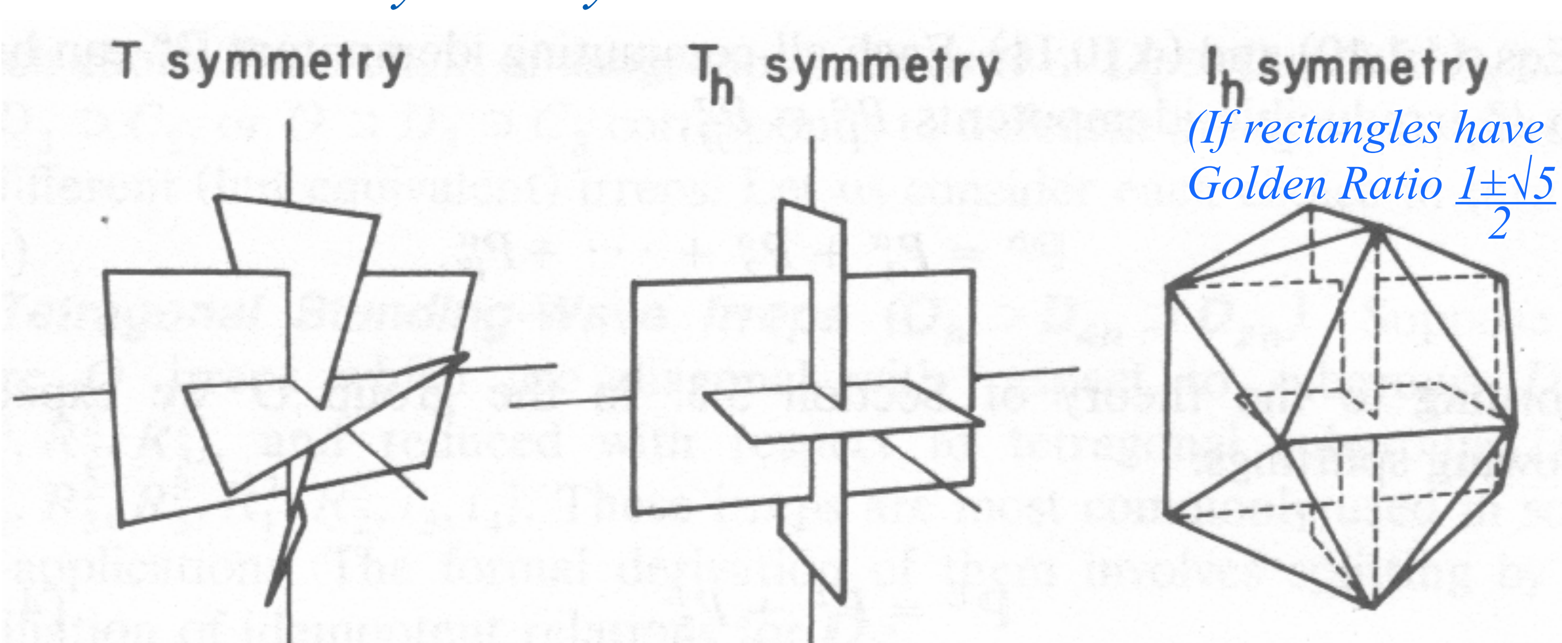
Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

Octahedral group O operations





Tetrahedral symmetry becomes Icosahedral



Int.J.Mol.Sci p.62.

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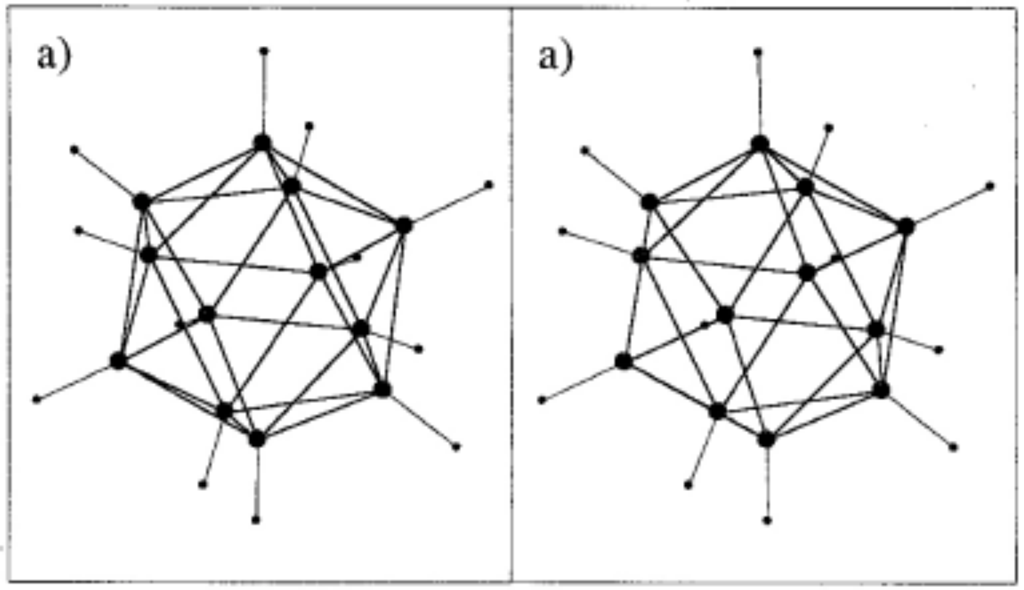
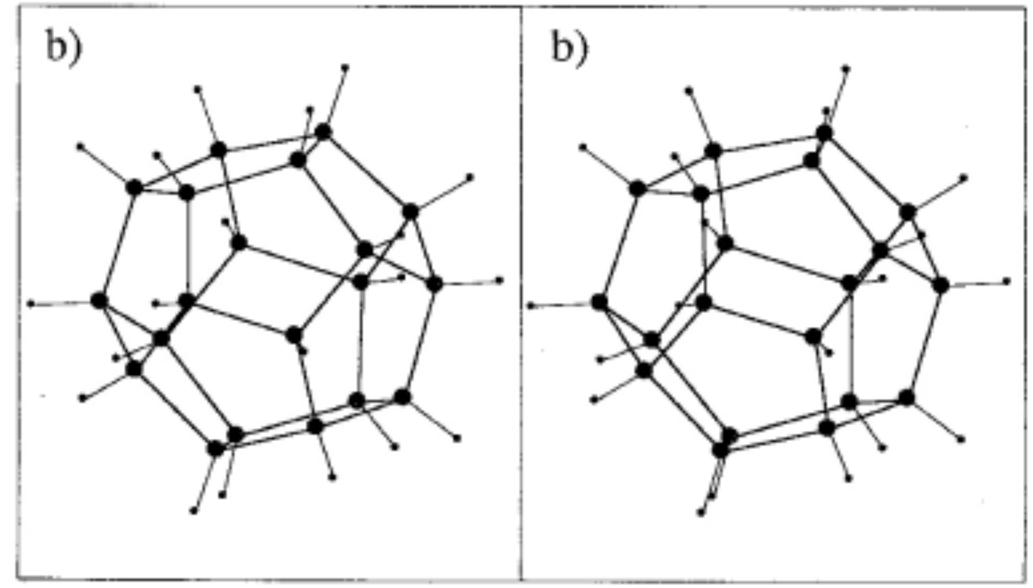
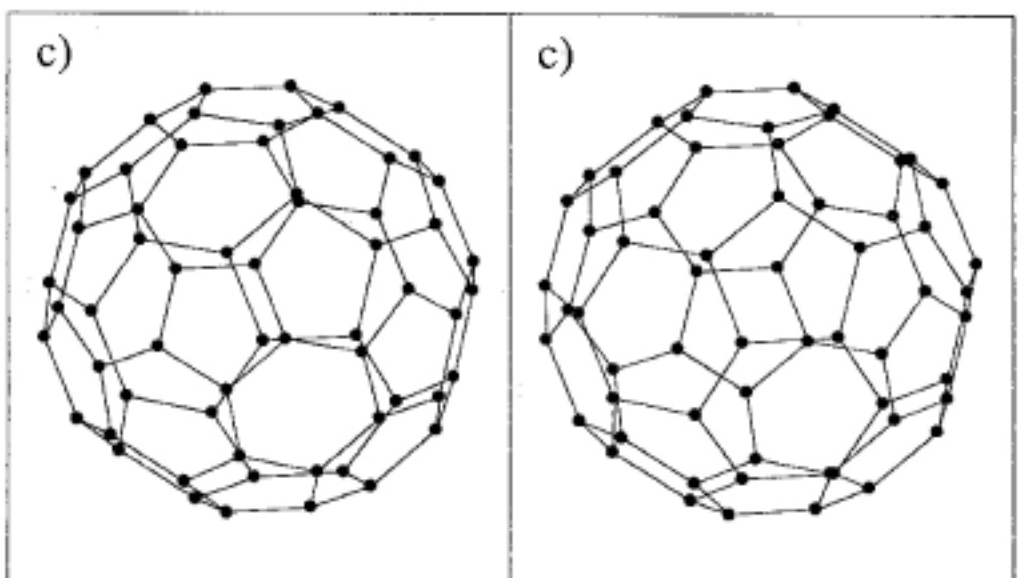
Three famous (but rare) molecules with I_h symmetry (in 3D "wall-eye" stereo)



$B_{12}H_{12}^{(-2)}$ Borohydride anion | $B_{12}H_{12}^{(-2)}$ Borohydride anion



$C_{20}H_{20}$ Dodecahedrane | $C_{20}H_{20}$ Dodecahedrane



"Bucky-ball" C_{60} Buckminsterfullerene | "Bucky-ball" C_{60} Buckminsterfullerene

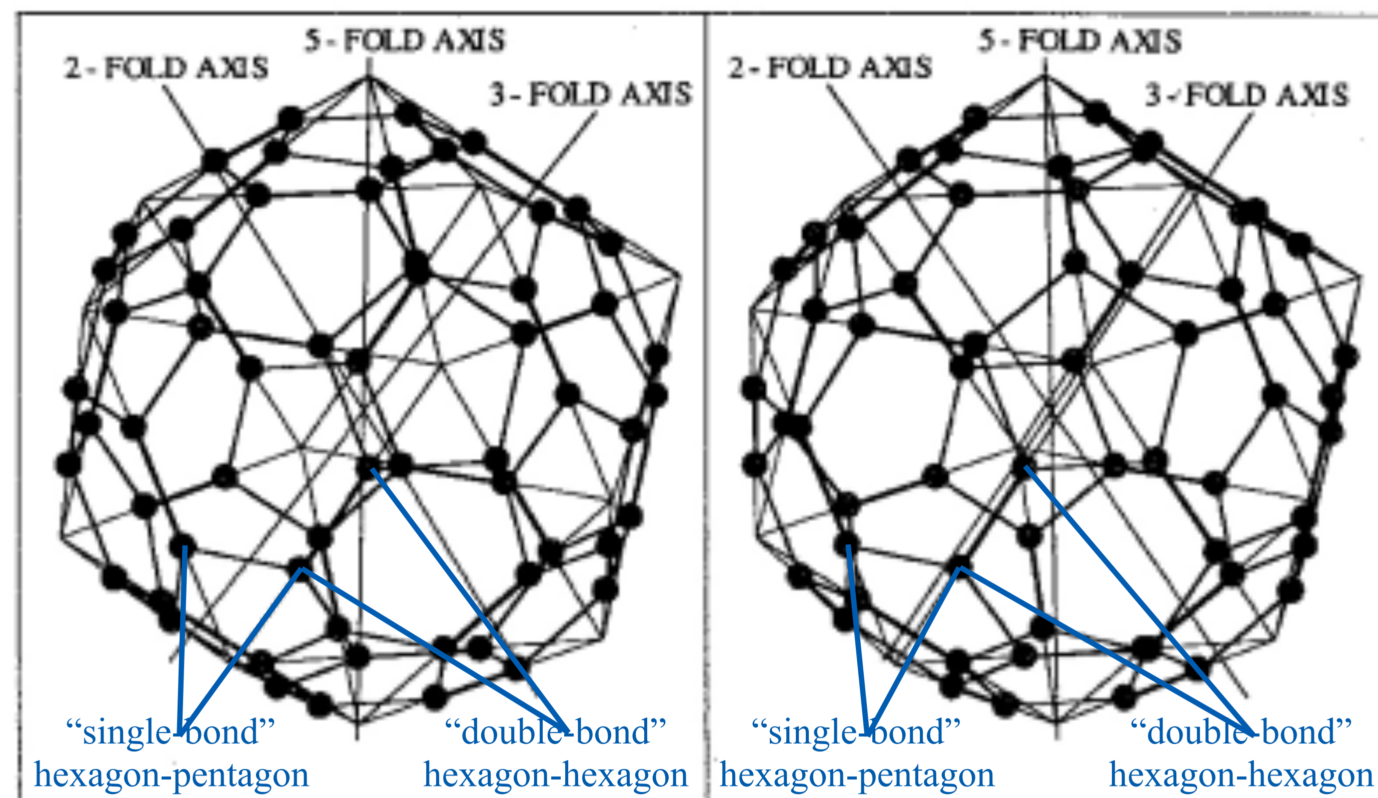


FIG. 2. Stereoscopic view of buckyball. "Double bonds" lie along the thick lines and "single bonds" lie along the thin lines. Carbon atoms are located at the vertices. An icosahedron is superimposed on the figure of buckyball to illustrate its icosahedral symmetry. Generic two, three, and fivefold symmetry axes are drawn and labeled.

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Weeks,Harter JCP90 pdf p.2

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Are there Buckyballs at the University of Arkansas?

Are there Buckyballs
at the
University of Arkansas?

Yes, Two of them!

Visit the
χω=ΧΩ
Greek Theatre

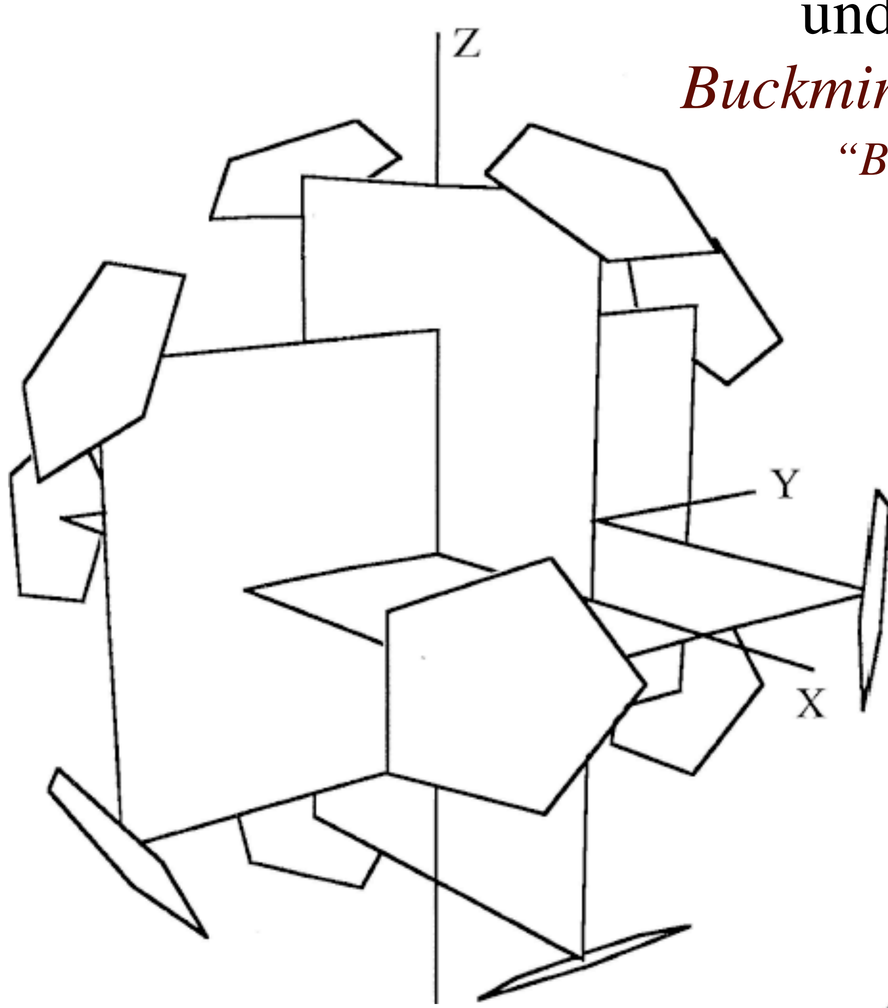
Three *Golden* rectangles

(Ratio: *(√5+1)/2 : 1=1.618...)*

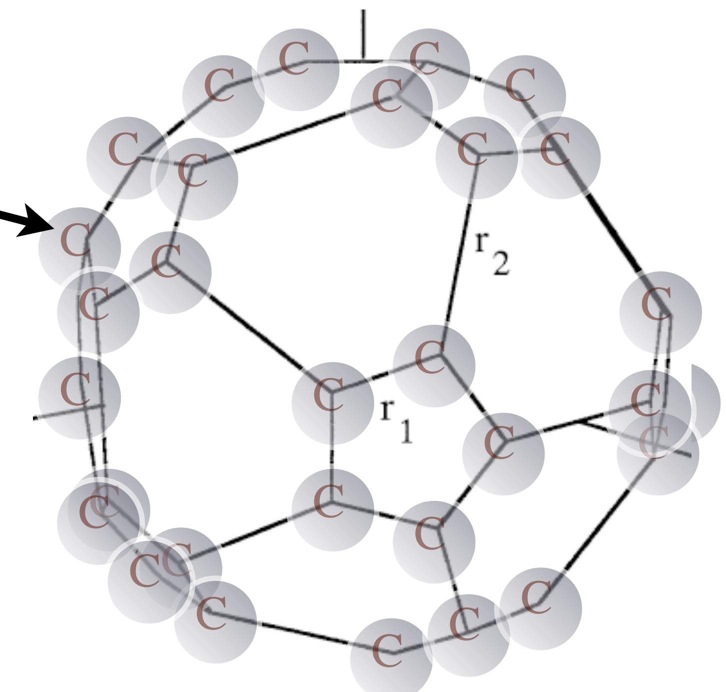
underlie C_{60}

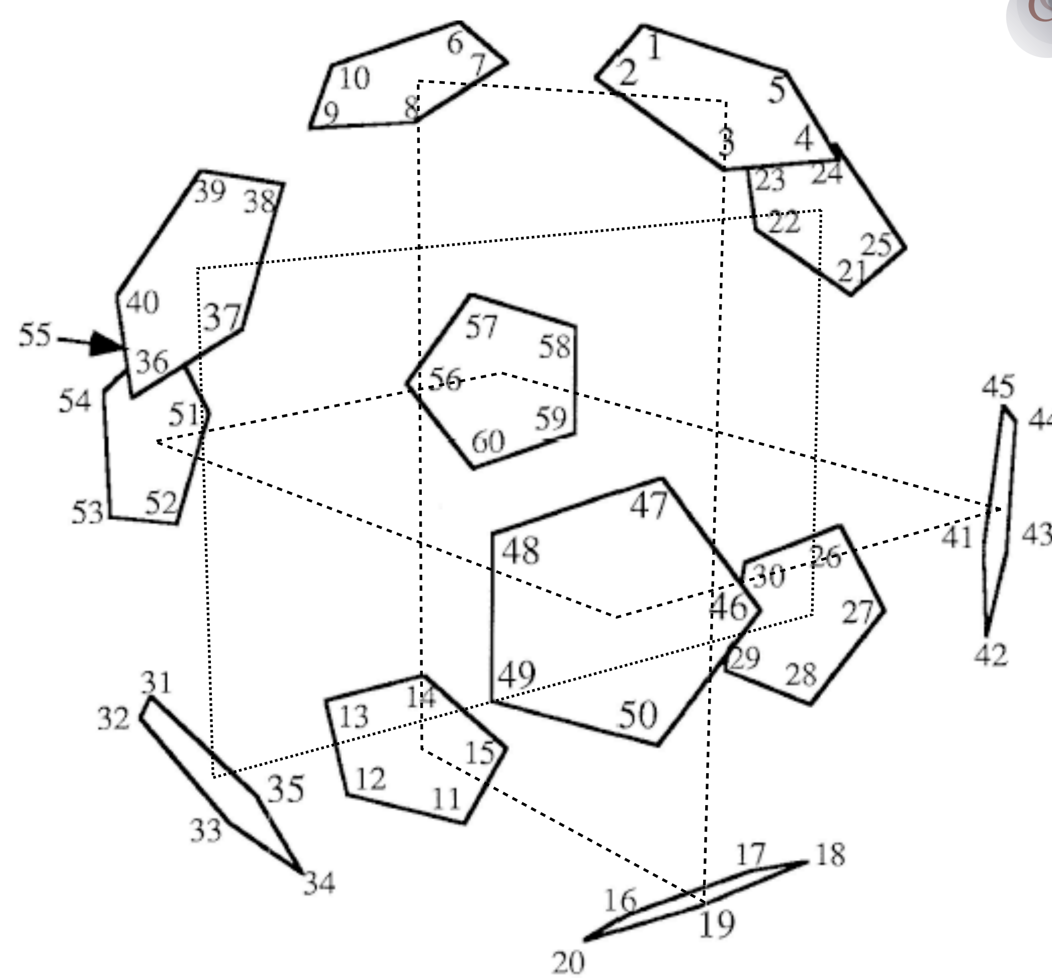
Buckminsterfullerene

"Buckyball"



60 C atoms:
one C at each
vertex
of a
Soccerball





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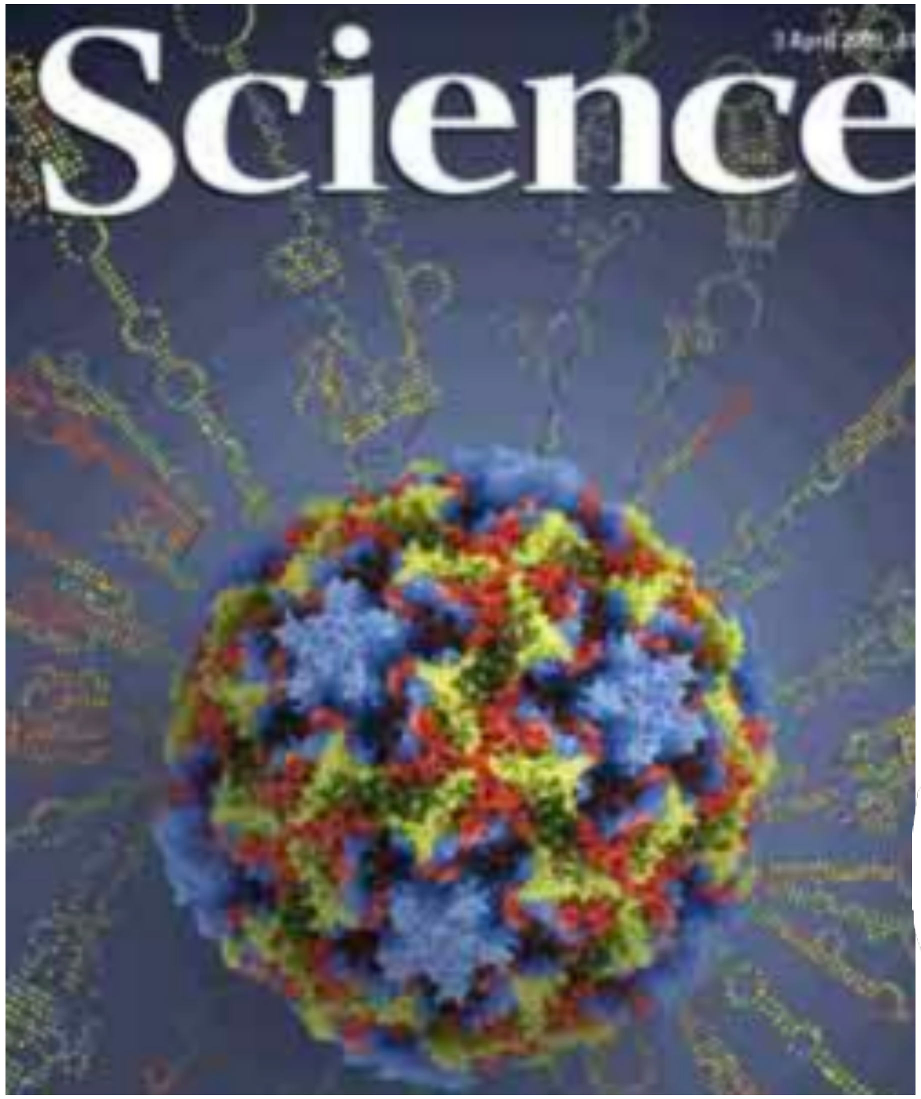
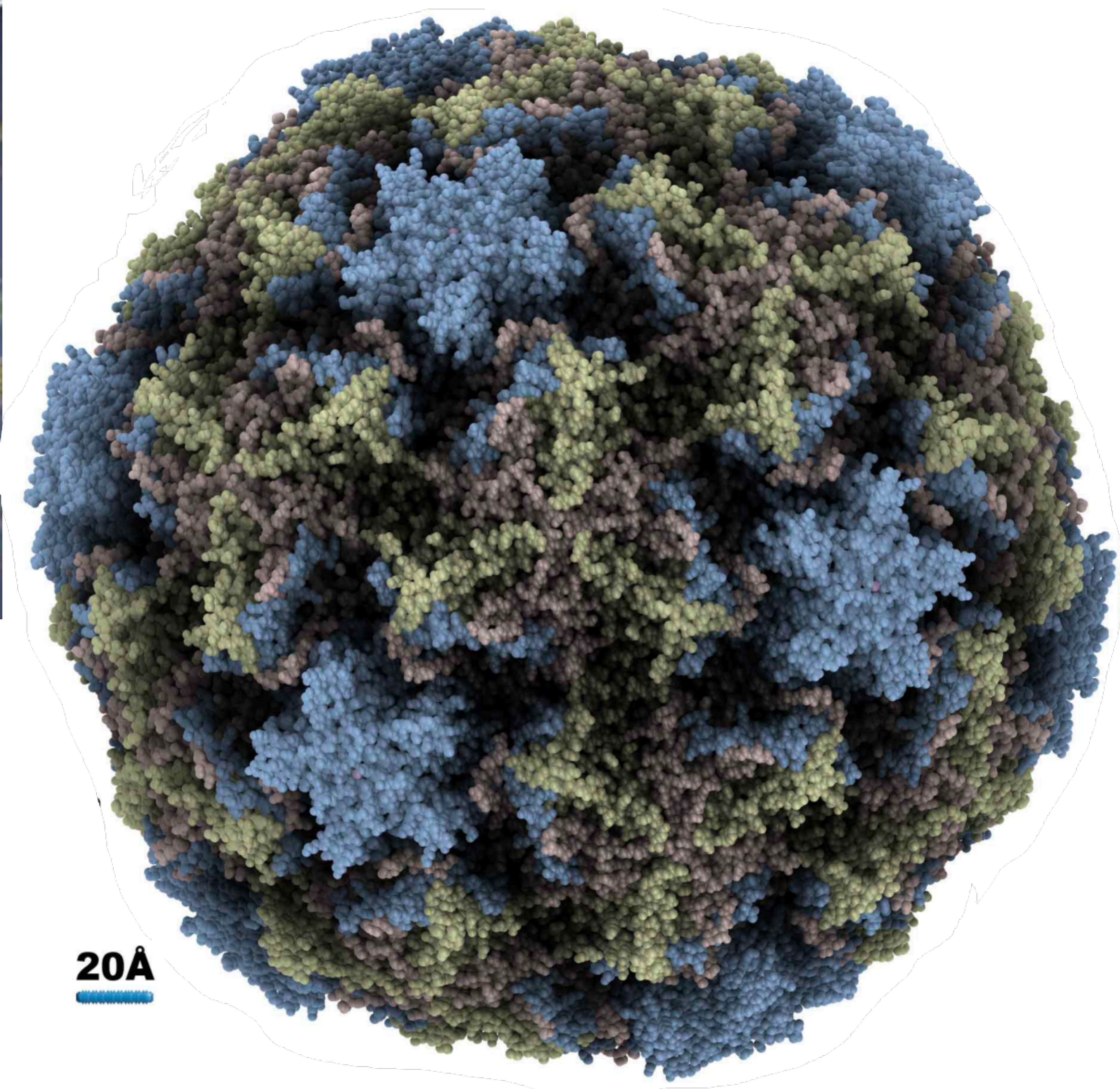
See Virology



Human rhinovirus 3
PDB ID: 1rhi

Zhao, R., Pevear, D.C., Kremer, M.J., Giranda, V.L., Kofron, J.A., Kuhn, R.J., Rossmann, M.G. (1996) *Human rhinovirus 3 at 3.0 Å resolution.* Structure 4: 1205-1220

A cause (one of many) of the Common Cold.



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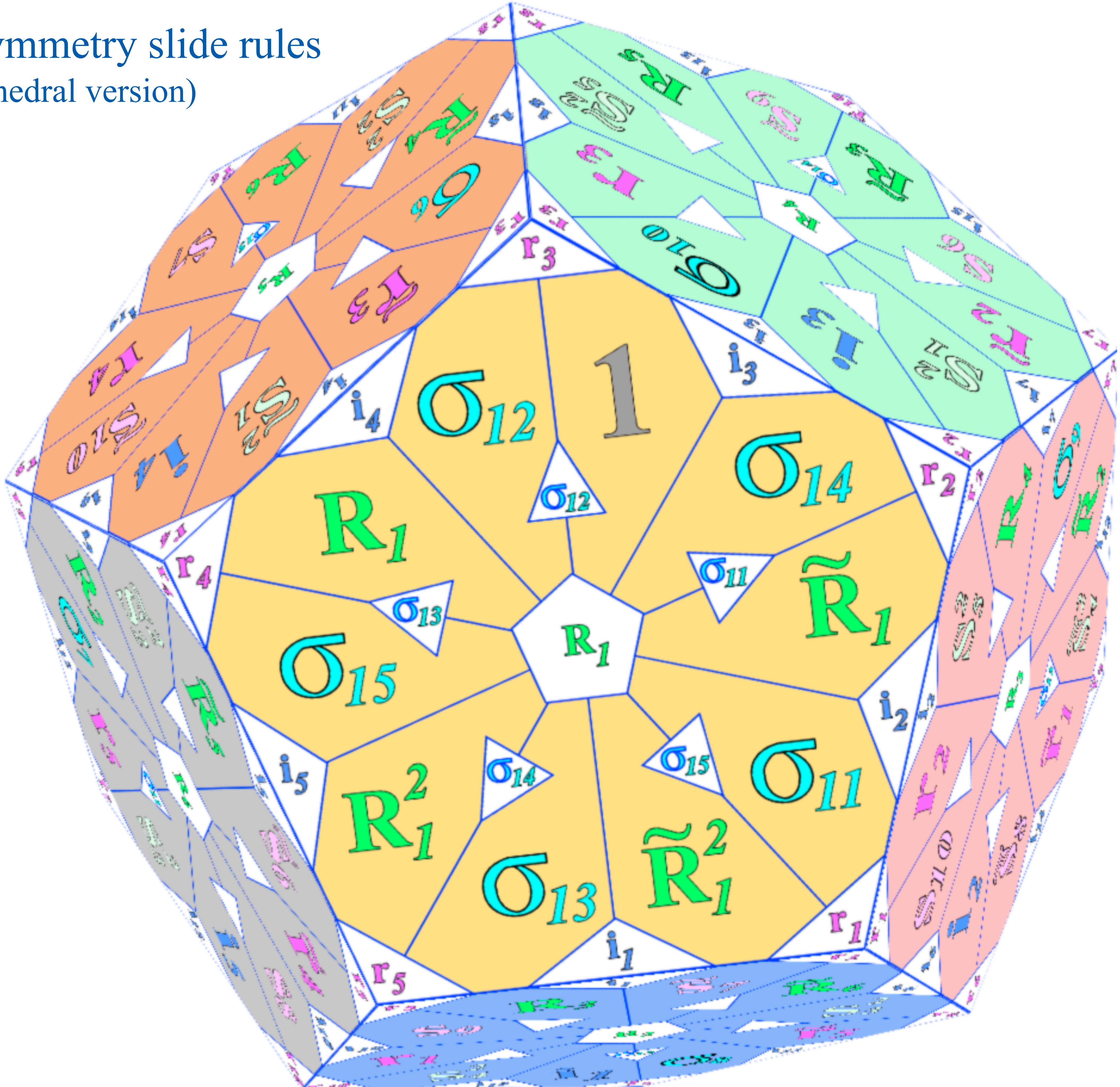
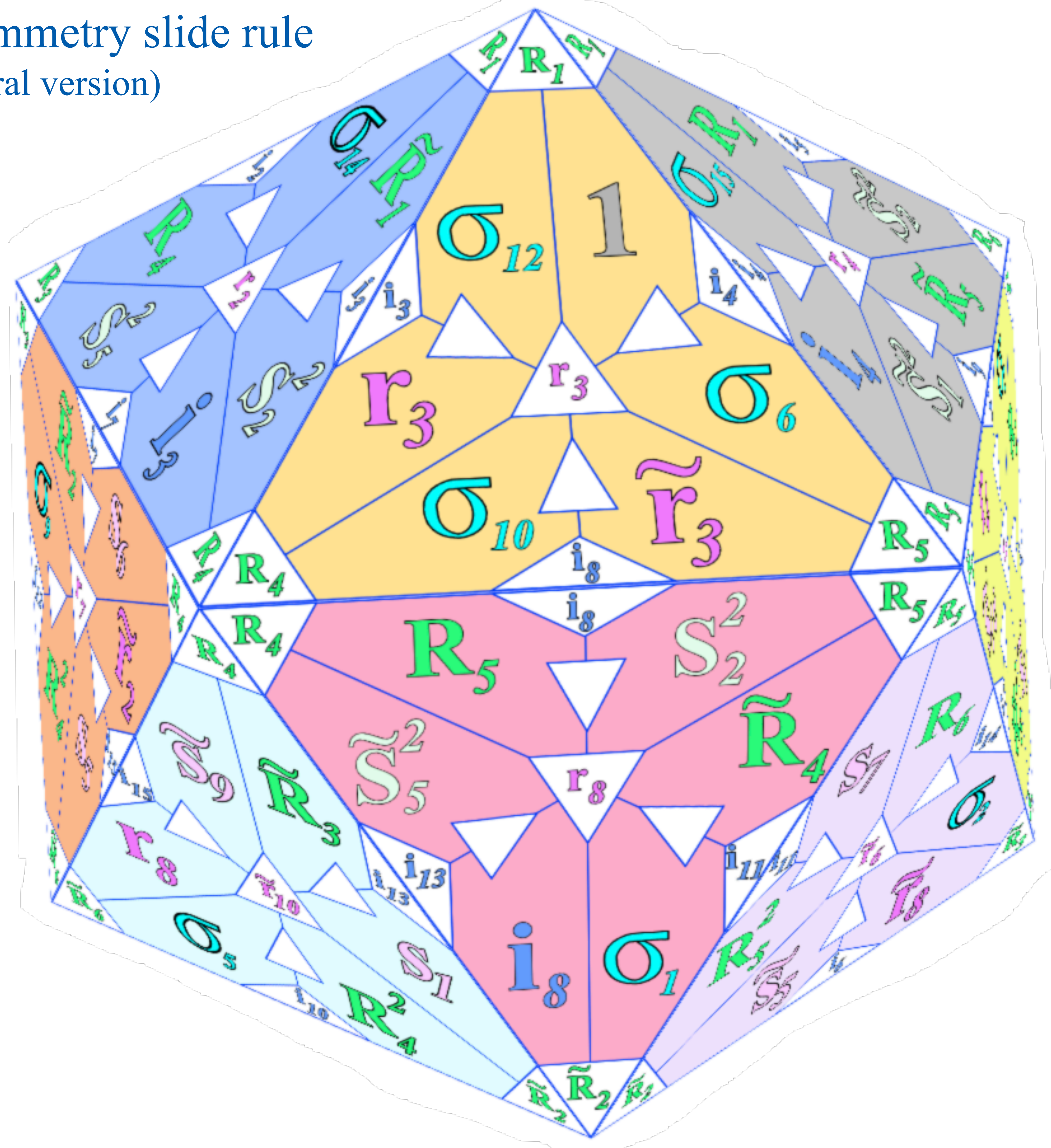
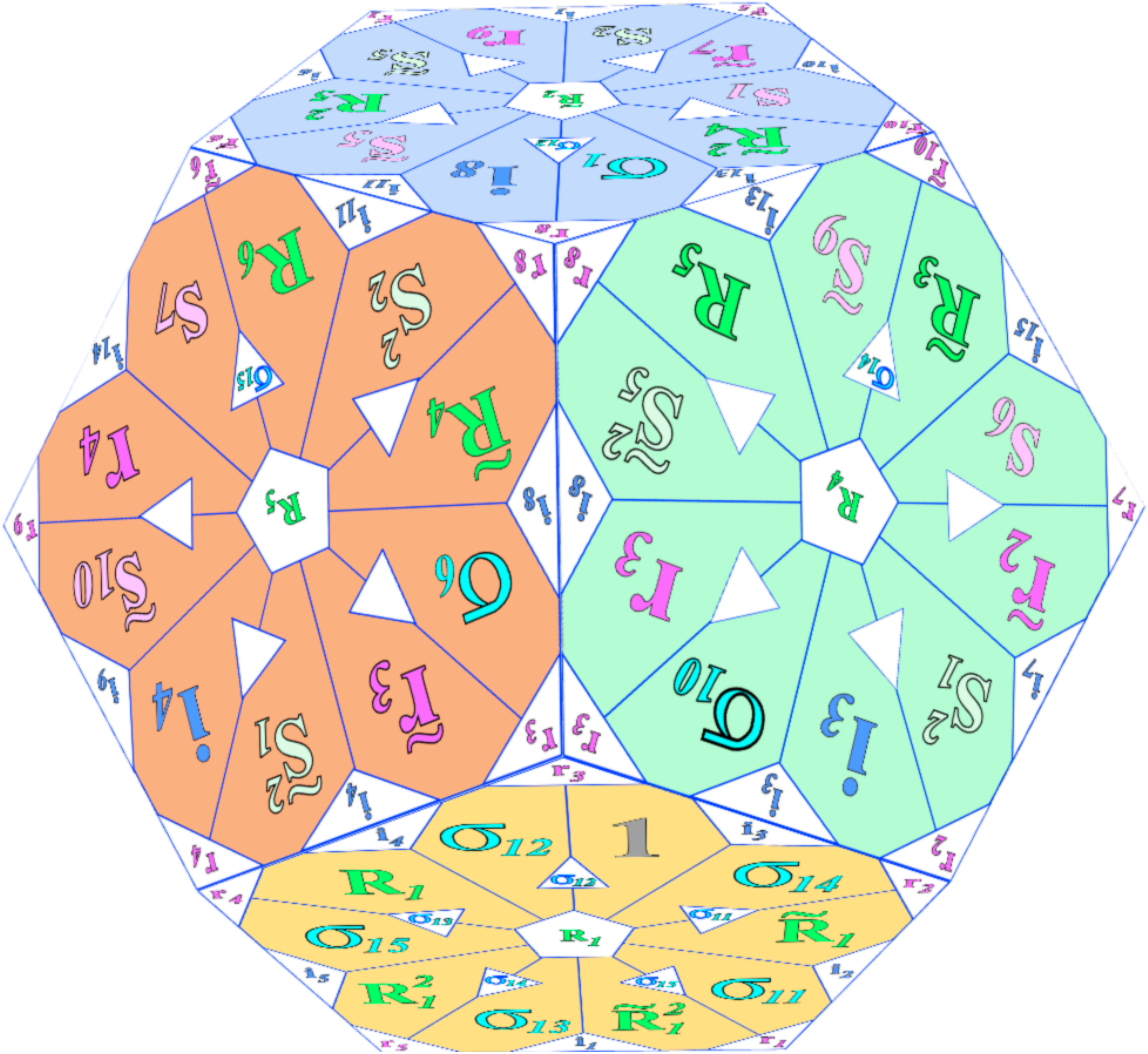


$I_h \supset I$ Symmetry slide rule
(Icosahedral version)



Here is a link to the new scenario at: https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=OhXY6



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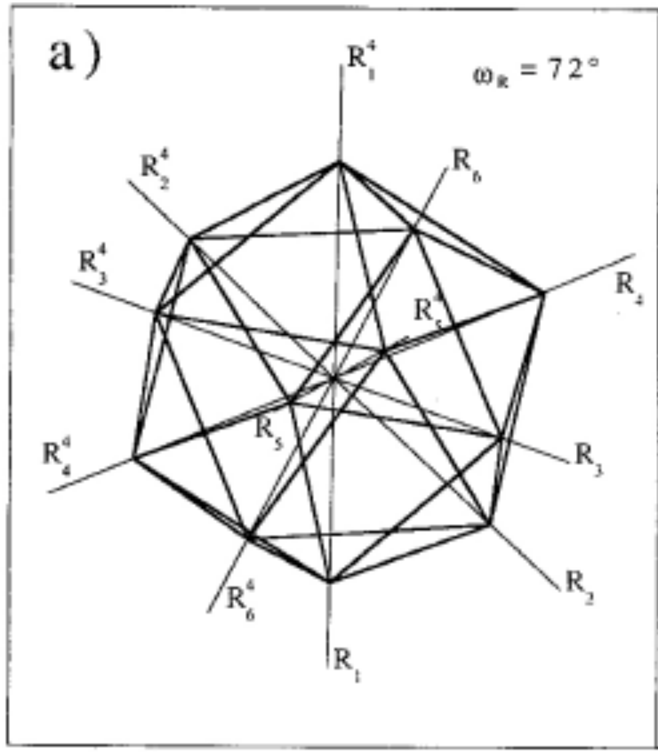
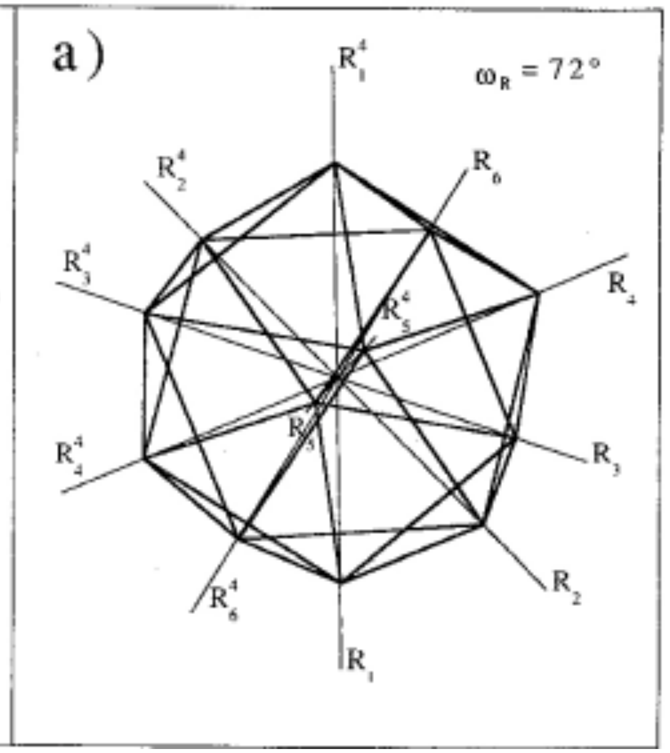
Some history of C_{60} discoveries

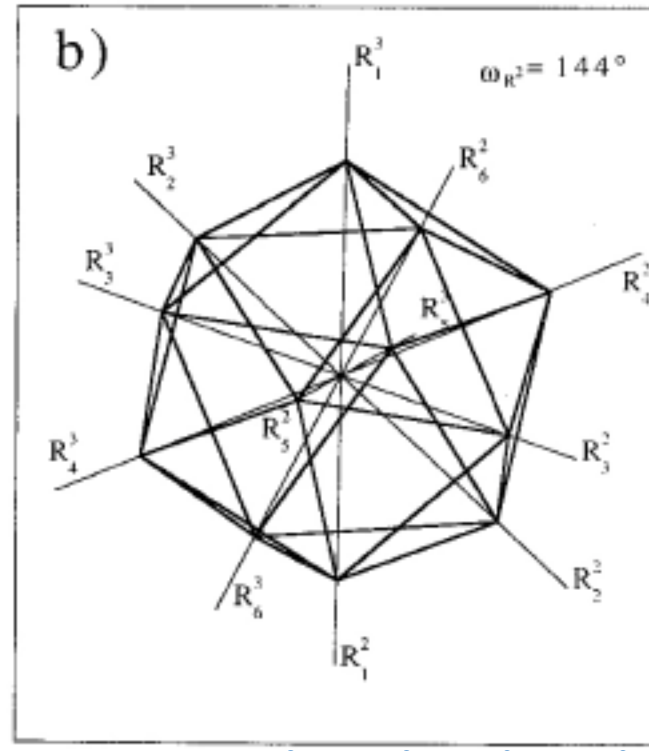
Icosahedral rotational operation classes in subgroup $I\subset I_h$ of $I_h=I\times C_i=I\times\{\mathbf{1},\mathbf{I}\}$



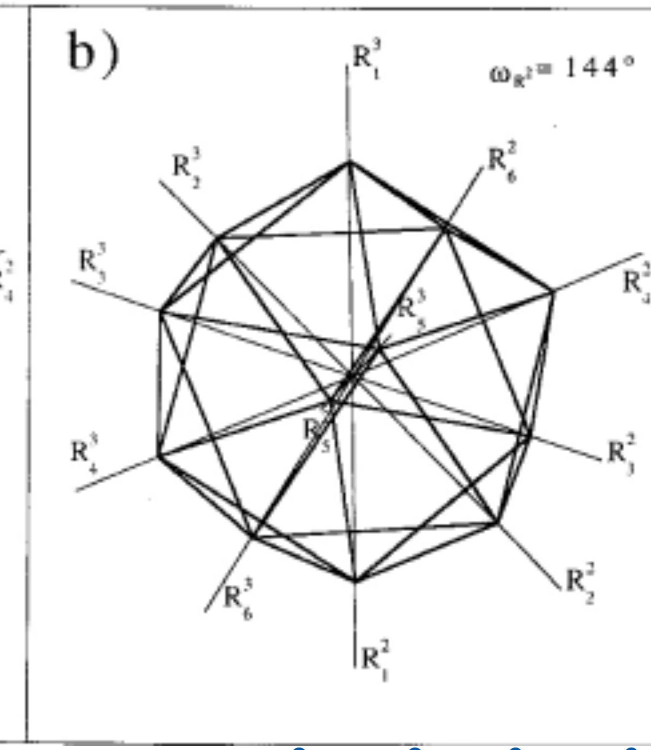
$\pm 72°$ $\mathbf{R}_1..\mathbf{R}_6,\mathbf{R}_1{}^4..\mathbf{R}_6{}^4$
(1_5) and (4_5) class



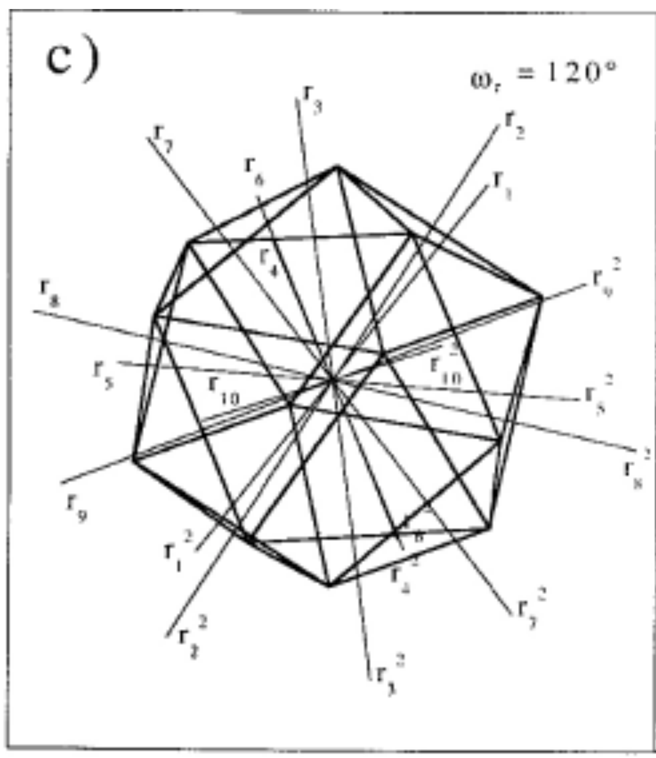
$\pm 72°$ $\mathbf{R}_1..\mathbf{R}_6,\mathbf{R}_1{}^4..\mathbf{R}_6{}^4$
(1_5) and (4_5) class



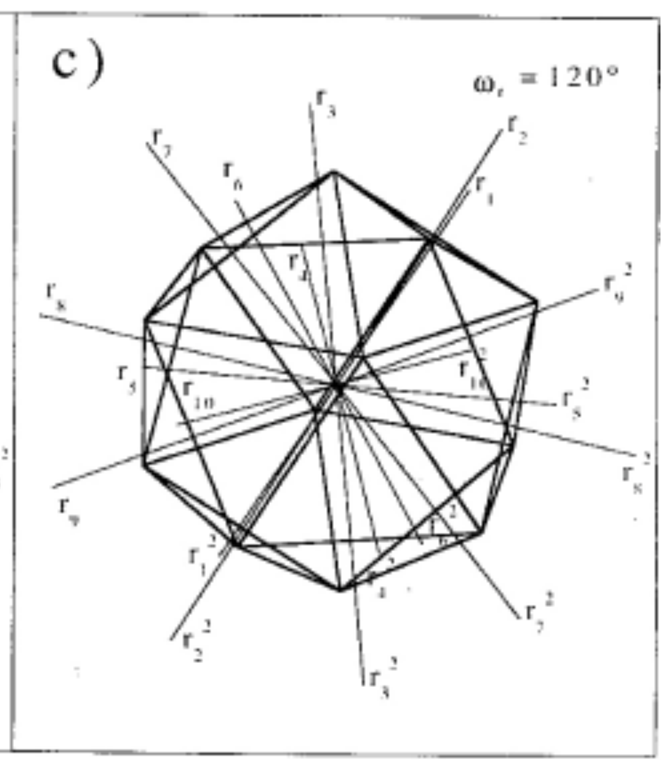
$\pm 144°$ $\mathbf{R}_1{}^2..\mathbf{R}_6{}^2,\mathbf{R}_1{}^3..\mathbf{R}_6{}^3$
(2_5) and (3_5) class



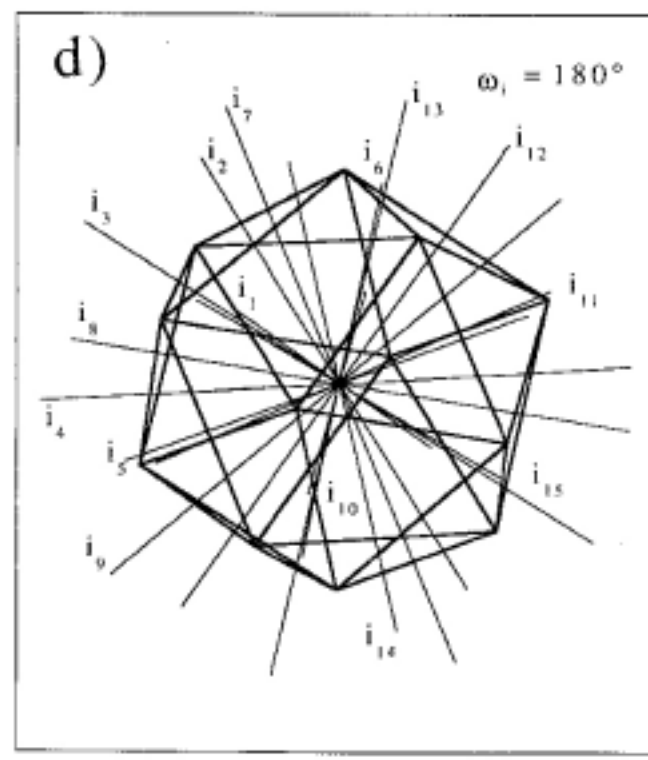
$\pm 144°$ $\mathbf{R}_1{}^2..\mathbf{R}_6{}^2,\mathbf{R}_1{}^3..\mathbf{R}_6{}^3$
(2_5) and (3_5) class



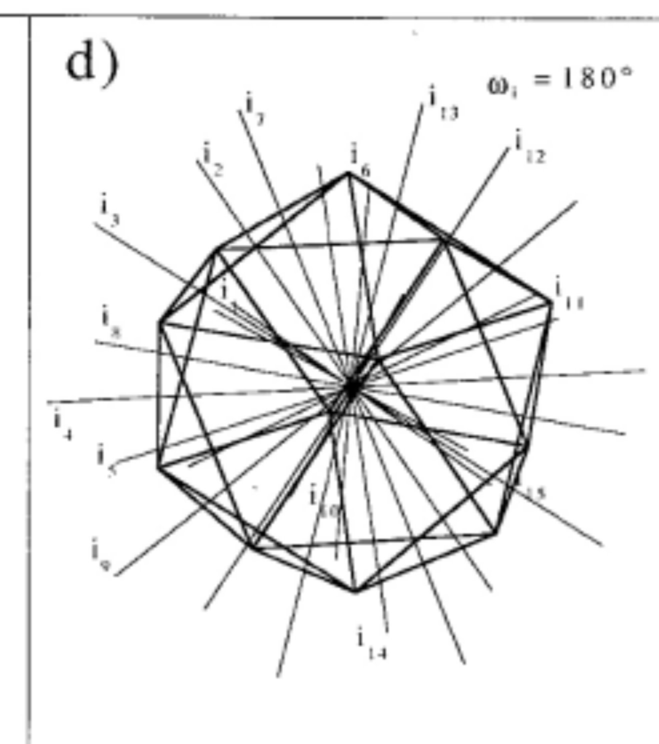
$\pm 120°$ $\mathbf{r}_1..\mathbf{r}_{10},\mathbf{r}_1{}^2..\mathbf{r}_{10}{}^2$
(1_3) and (2_3) class



$\pm 120°$ $\mathbf{r}_1..\mathbf{r}_{10},\mathbf{r}_1{}^2..\mathbf{r}_{10}{}^2$
(1_3) and (2_3) class



$\pm 180°$ $\mathbf{i}_1..\mathbf{i}_7,\mathbf{i}_8..\mathbf{i}_{15}$
(0_2) and (1_2) class



$\pm 180°$ $\mathbf{i}_1..\mathbf{i}_7,\mathbf{i}_8..\mathbf{i}_{15}$
(0_2) and (1_2) class

Weeks,Harter JCP90 pdf p.3

0° Identity **1**

(0_5) class

±72° $\mathbf{R_1..R_6, R_1^4..R_6^4}$

(1_5) and (4_5) class

(12 members)

±*144*° $\mathbf{R_1^2..R_6^2, R_1^3..R_6^3}$

(2_5) and (3_5) class

(12 members)

±*120*° $\mathbf{r_1..r_{10}, r_1^2..r_{10}^2}$

(1_3) and (2_3) class

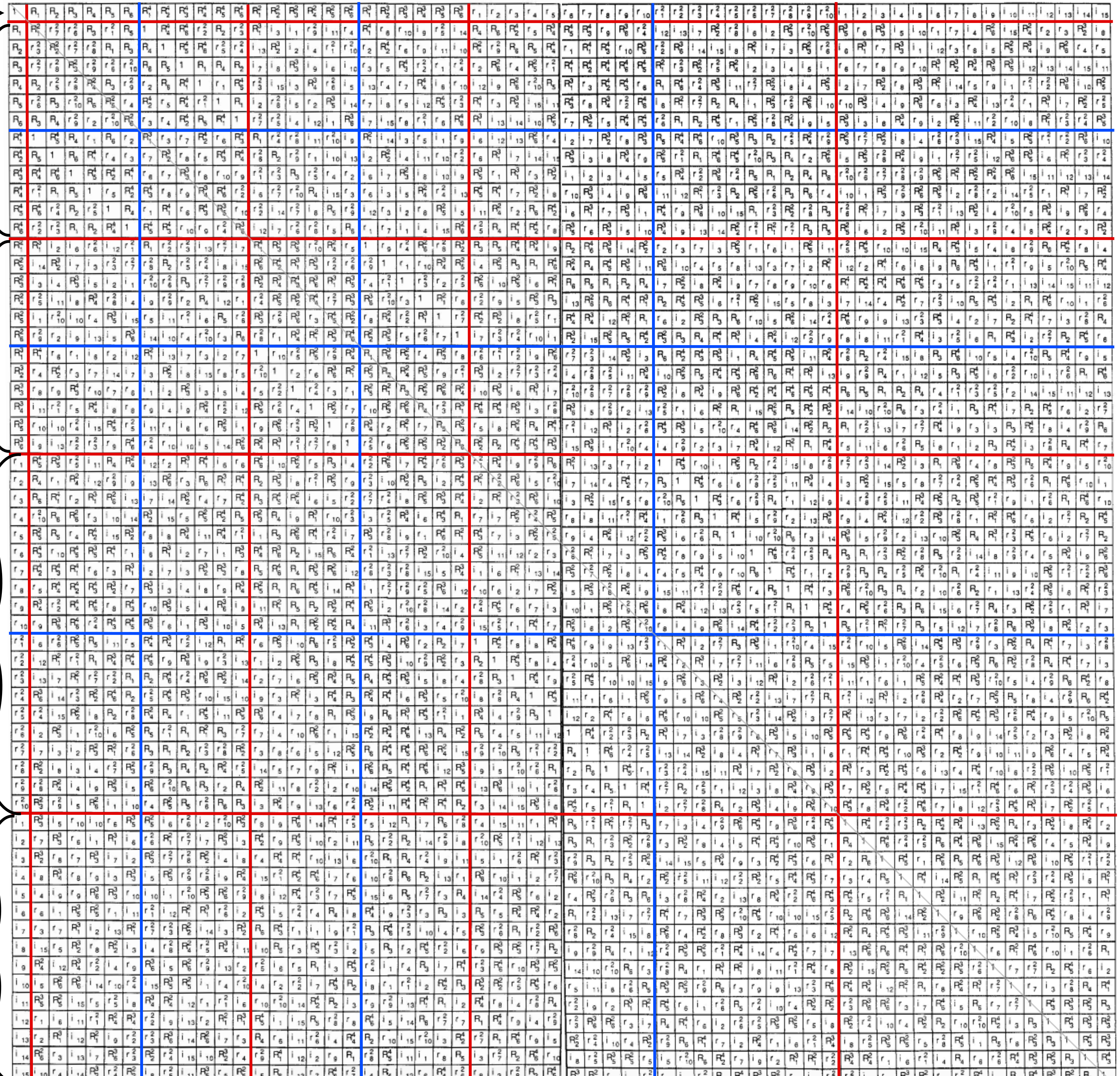
(20 members)

Product Table
Subgroup $I \subset I_h$

±*180*° $\mathbf{i_1..i_7, i_8..i_{15}}$

(0_2) and (1_2) class

(15 members)



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List of *Icosahedral I group operators* by class

Icosahedral {I} Class Structure			
$C_1 = 1$			
C_R	C_{R^2}	C_r	C_i
ω=72	ω=144	ω=120	ω=180
R_1	R_1^2	r_1	i_1
R_2	R_2^2	r_2	i_2
R_3	R_3^2	r_3	i_3
R_4	R_4^2	r_4	i_4
R_5	R_5^2	r_5	i_5
R_6	R_6^2	r_6	i_6
R_1^4	R_1^3	r_7	i_7
R_2^4	R_2^3	r_8	i_8
R_3^4	R_3^3	r_9	i_9
R_4^4	R_4^3	r_{10}	i_{10}
R_5^4	R_5^3	r_1^2	i_{11}
R_6^4	R_6^3	r_2^2	i_{12}
		r_3^2	i_{13}
		r_4^2	i_{14}
		r_5^2	i_{15}
		r_6^2	
		r_7^2	
		r_8^2	
		r_9^2	
		r_{10}^2	

Weeks,Harter JCP90 pdf p.4

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Icosahedral {I} Class Structure

$C_1 = 1$			
C_R	C_{R^2}	C_r	C_i
ω=72	ω=144	ω=120	ω=180
R_1	R_1^2	r_1	i_1
R_2	R_2^2	r_2	i_2
R_3	R_3^2	r_3	i_3
R_4	R_4^2	r_4	i_4
R_5	R_5^2	r_5	i_5
R_6	R_6^2	r_6	i_6
R_1^4	R_1^3	r_7	i_7
R_2^4	R_2^3	r_8	i_8
R_3^4	R_3^3	r_9	i_9
R_4^4	R_4^3	r_{10}	i_{10}
R_5^4	R_5^3	r_1^2	i_{11}
R_6^4	R_6^3	r_2^2	i_{12}
		r_3^2	i_{13}
		r_4^2	i_{14}
		r_5^2	i_{15}
		r_6^2	
		r_7^2	
		r_8^2	
		r_9^2	
		r_{10}^2	

Icosahedral $\{I_h\}$ Class Structure

$C_I = I$			
C_ρ	C_{ρ^2}	C_η	C_σ
$I\ R_1 = \rho_1$	$I\ R_1^2 = \rho_1^2$	$I\ r_1 = \eta_1$	$I\ i_1 = \sigma_1$
$I\ R_2 = \rho_2$	$I\ R_2^2 = \rho_2^2$	$I\ r_2 = \eta_2$	$I\ i_2 = \sigma_2$
$I\ R_3 = \rho_3$	$I\ R_3^2 = \rho_3^2$	$I\ r_3 = \eta_3$	$I\ i_3 = \sigma_3$
$I\ R_4 = \rho_4$	$I\ R_4^2 = \rho_4^2$	$I\ r_4 = \eta_4$	$I\ i_4 = \sigma_4$
$I\ R_5 = \rho_5$	$I\ R_5^2 = \rho_5^2$	$I\ r_5 = \eta_5$	$I\ i_5 = \sigma_5$
$I\ R_6 = \rho_6$	$I\ R_6^2 = \rho_6^2$	$I\ r_6 = \eta_6$	$I\ i_6 = \sigma_6$
$I\ R_1^4 = \rho_1^4$	$I\ R_1^3 = \rho_1^3$	$I\ r_7 = \eta_7$	$I\ i_7 = \sigma_7$
$I\ R_2^4 = \rho_2^4$	$I\ R_2^3 = \rho_2^3$	$I\ r_8 = \eta_8$	$I\ i_8 = \sigma_8$
$I\ R_3^4 = \rho_3^4$	$I\ R_3^3 = \rho_3^3$	$I\ r_9 = \eta_9$	$I\ i_9 = \sigma_9$
$I\ R_4^4 = \rho_4^4$	$I\ R_4^3 = \rho_4^3$	$I\ r_{10} = \eta_{10}$	$I\ i_{10} = \sigma_{10}$
$I\ R_5^4 = \rho_5^4$	$I\ R_5^3 = \rho_5^3$	$I\ r_1^2 = \eta_1^2$	$I\ i_{11} = \sigma_{11}$
$I\ R_6^4 = \rho_6^4$	$I\ R_6^3 = \rho_6^3$	$I\ r_2^2 = \eta_2^2$	$I\ i_{12} = \sigma_{12}$
		$I\ r_3^2 = \eta_3^2$	$I\ i_{13} = \sigma_{13}$
		$I\ r_4^2 = \eta_4^2$	$I\ i_{14} = \sigma_{14}$
		$I\ r_5^2 = \eta_5^2$	$I\ i_{15} = \sigma_{15}$
		$I\ r_6^2 = \eta_6^2$	
		$I\ r_7^2 = \eta_7^2$	
		$I\ r_8^2 = \eta_8^2$	
		$I\ r_9^2 = \eta_9^2$	
		$I\ r_{10}^2 = \eta_{10}^2$	

I_h Class Operators

$$cR = \sum_{n=1}^{6} R_n + R_n^4 \qquad c\rho = I\ cR$$

$$cR^2 = \sum_{n=1}^{6} R_n^2 + R_n^3 \qquad c\rho^2 = I\ cR^2$$

$$cr = \sum_{n=1}^{10} r_n + r_n^2 \qquad c\eta = I\ cr$$

$$ci = \sum_{n=1}^{15} i_n \qquad c\sigma = I\ ci$$

Complete list of *Icosahedral I_h group operators* by class

Weeks,Harter JCP90 pdf p.4

AMOP
reference links
on pages 2-4

5.08.18 class 29: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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Icosahedral subgroup $I \subset I_h$ isomorphic to even-permutation group $A_5 \subset S_5$

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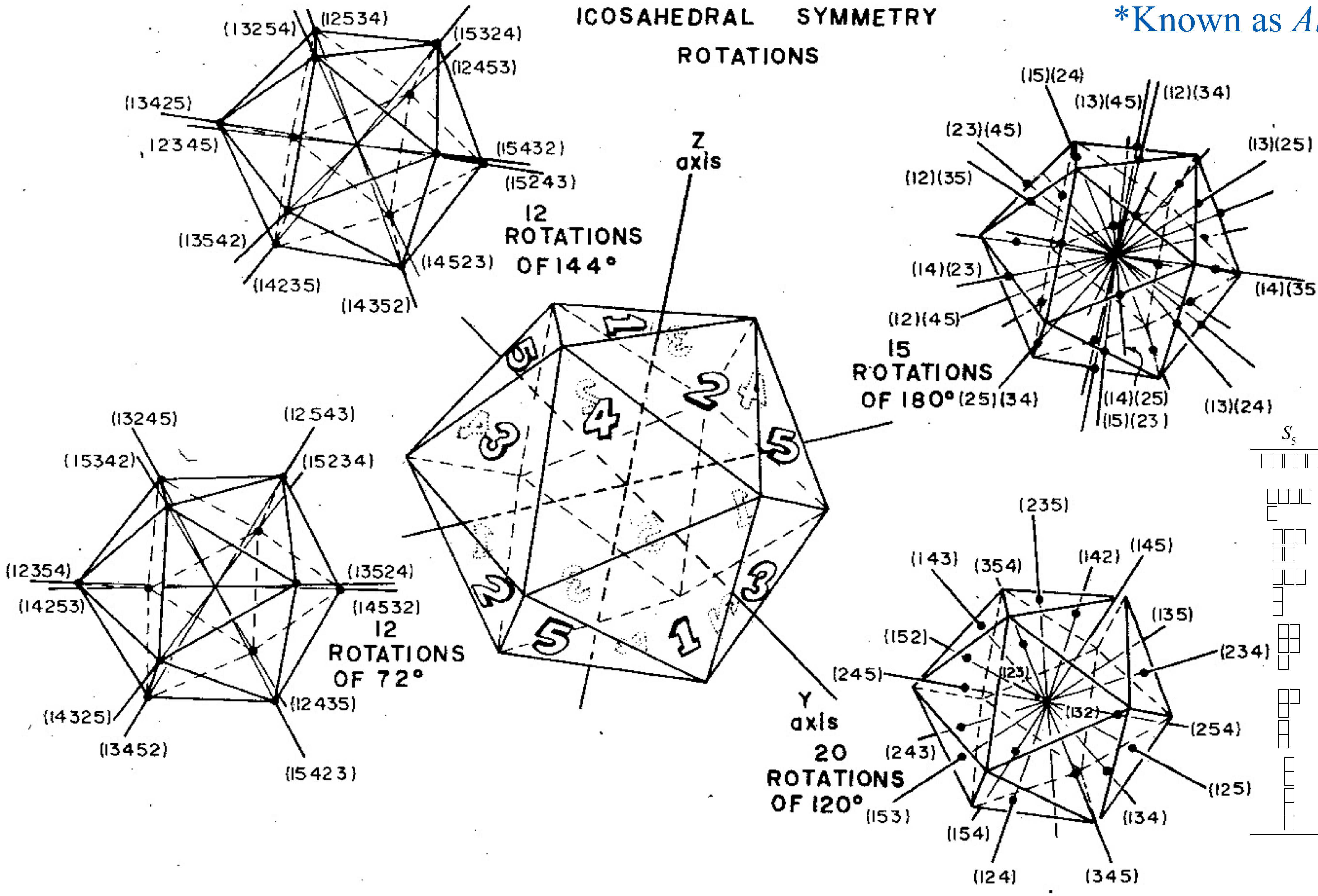
Icosahedral subgroup $I \subset I_h$ isomorphic to even-permutation* group $A_5 \subset S_5$

*Known as *Alternating Group*



S_5 Characters

S_5	1^5	21^3	2^21	31^2	32	41	5
□□□□□	1	1	1	1	1	1	1
□□□□ □	4	2	0	1	−1	0	−1
□□□ □□	5	−1	1	−1	−1	1	0
□□□ □ □	6	0	−2	0	0	0	1
□□ □□ □	5	1	1	−1	1	−1	0
□□ □ □ □	4	−2	0	1	1	0	−1
□ □ □ □ □	1	−1	1	1	−1	−1	1

Odd=red Even=green

W.Harter, N.DosSantos, Double-Group Theory on the Half-Shell I ,Am. J. Phys. 46, 251 (1978) pdf p.9

https://modphys.hosted.uark.edu/pdfs/Journal_Pdfs/Doublegroup_theory_on_the_halfshell_and_the_twolevel_system_I_Rotation_and_half_integral_spin_states_-_Santos_-_AJP_-_harter1978.pdf

https://modphys.hosted.uark.edu/pdfs/Journal_Pdfs/Doublegroup_theory_on_the_halfshell_and_the_twolevel_system_II_Optical_polarization_-_Santos_-_AJP_-_harter_-_1978.pdf

The symmetry group of "Buckyball" C_{60}

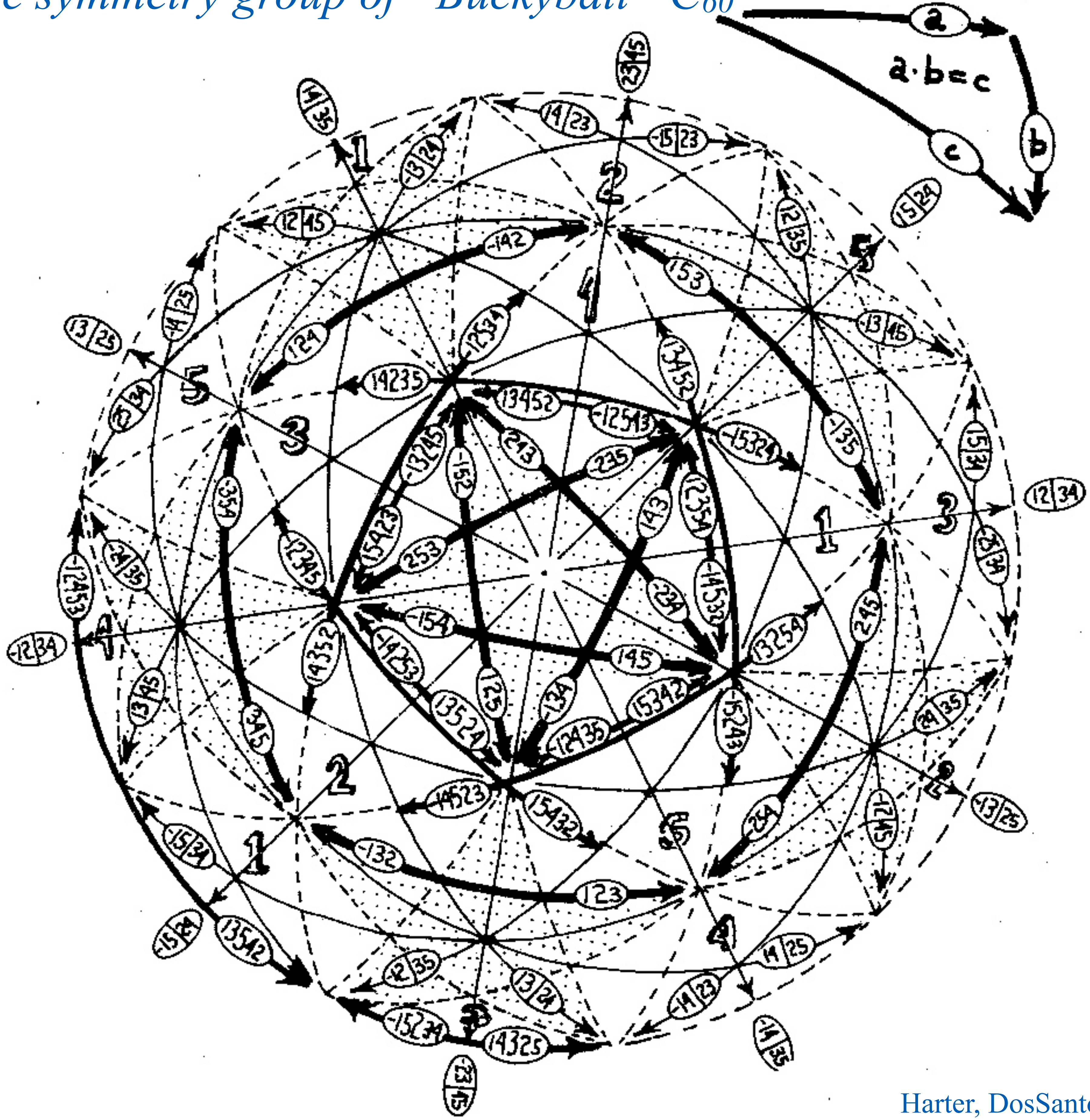


Fig. 10. Icosahedral vector addition nomogram.

S_5 Characters

S_5	1^5	21^3	2^21	31^2	32	41	5
□□□□□	1	1	1	1	1	1	1
□□□□ □	4	2	0	1	−1	0	−1
□□□ □□	5	−1	1	−1	−1	1	0
□□□ □ □	6	0	−2	0	0	0	1
□□ □□ □	5	1	1	−1	1	−1	0
□□ □ □ □	4	−2	0	1	1	0	−1
□ □ □ □ □	1	−1	1	1	−1	−1	1

Odd=red Even=green

Harter, DosSantos, AJP(1978) pdf p.10

Hamilton-turn-arcs for "Buckyball" C_{60}

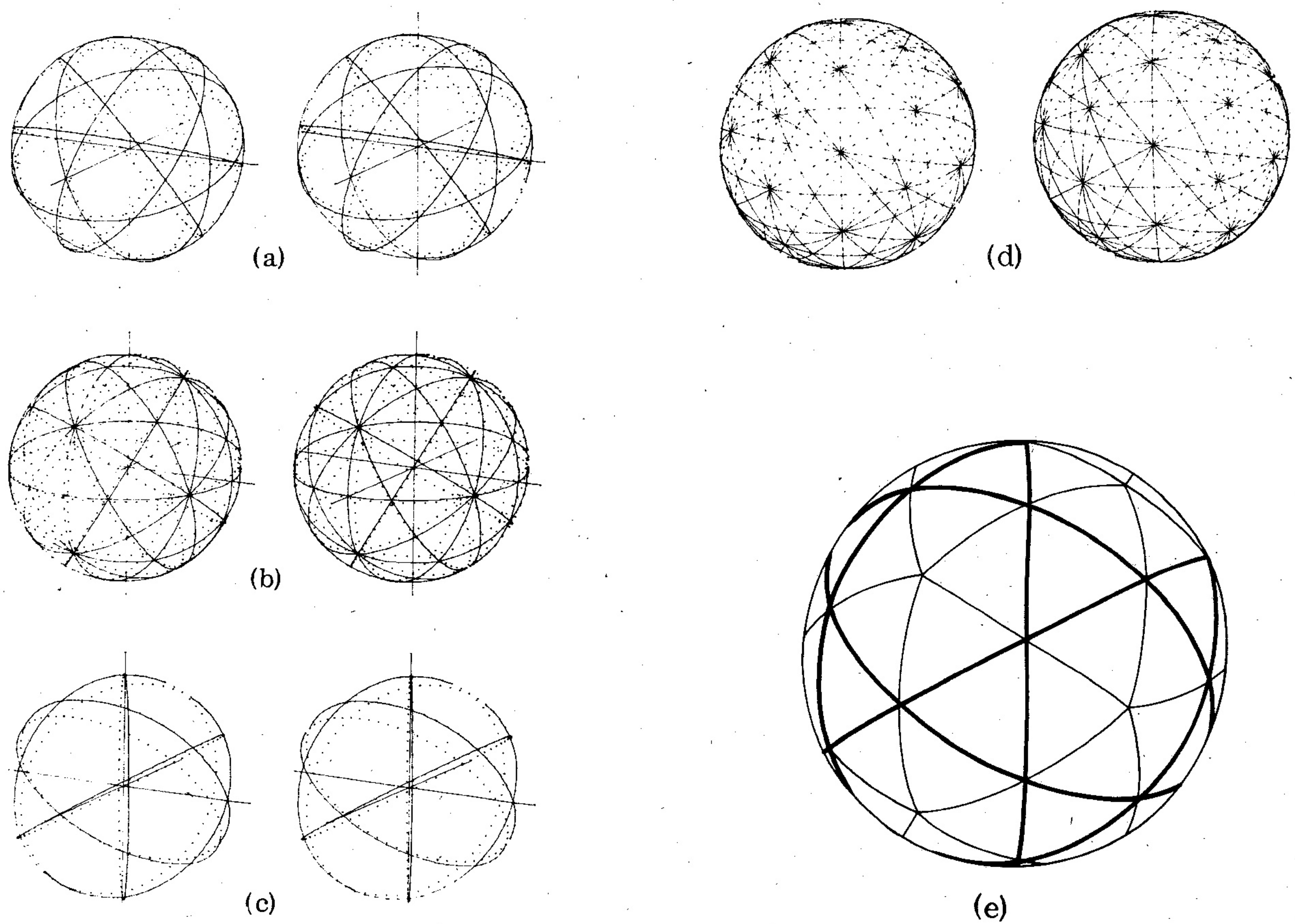


Fig. 9. Hamilton arcs for icosahedral symmetry. Stereo drawings of arcs paths for (a) 120°, (b) 180°, (c) 72° and 144° rotations all show icosahedral symmetry. All the arcs are drawn together in (d). This forms the icosahedral "lattice" which is projected to make the nomogram (Fig. 10). (e) The 72° arc paths are selected parts of the 180° arc paths form the elementary geodesic dome structure of Fuller.

W.Harter, N.DosSantos, Double-Group Theory on the Half-Shell I and II ,Am. J. Phys. 46, 251 (1978)

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Cartesian coordination at Carbon atom vertices

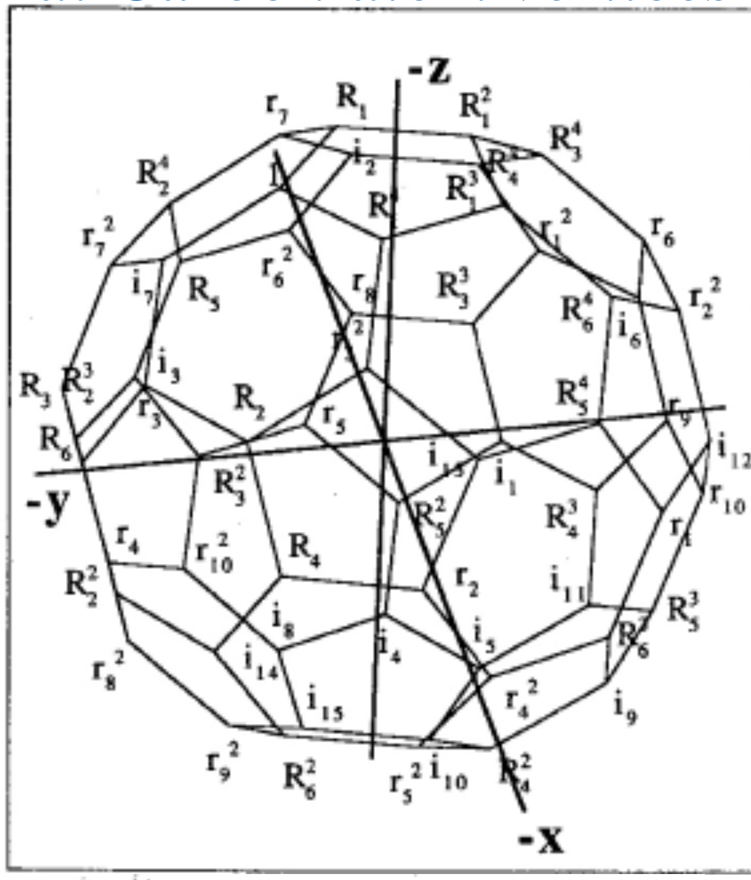


FIG. 6. Icosahedral vertex labels and the body-fixed *x*, *y*, and *z* axes.

Cartesian coordination at Carbon atom vertices

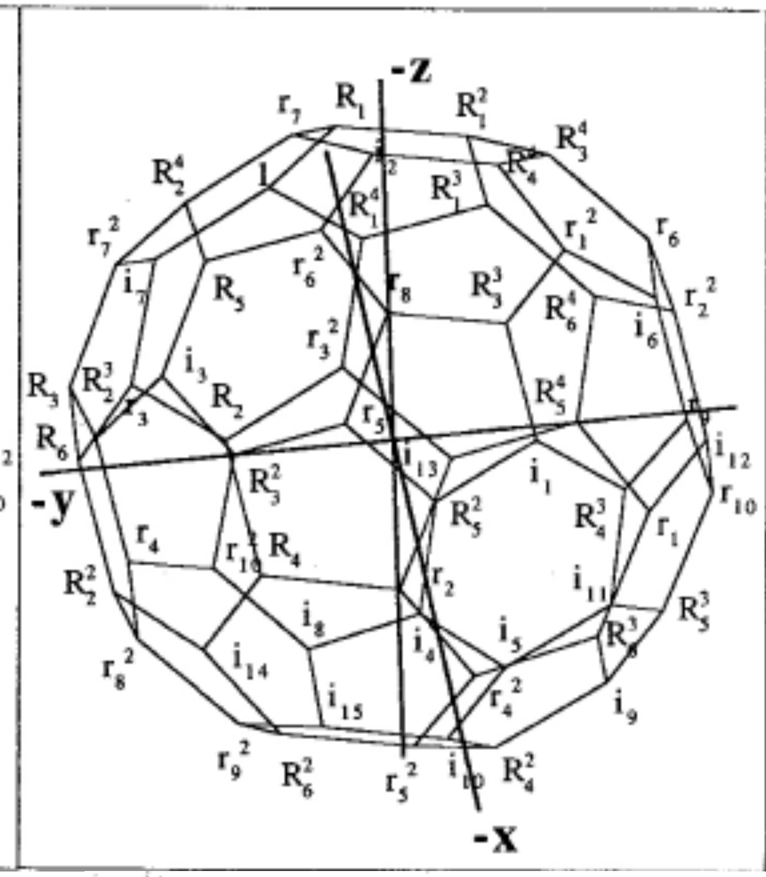
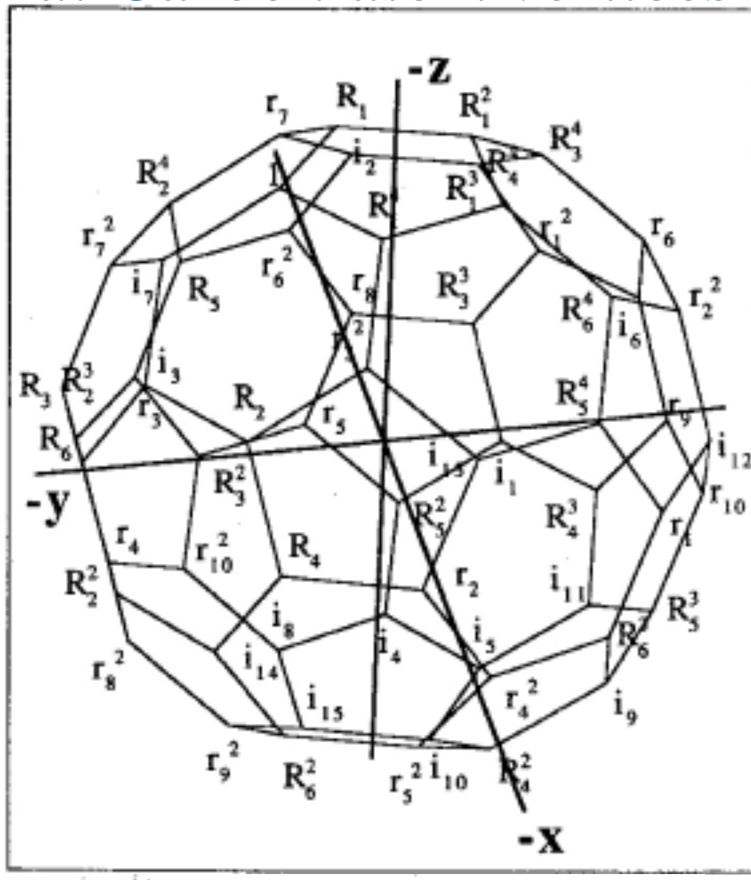


FIG. 6. Icosahedral vertex labels and the body-fixed *x*, *y*, and *z* axes.

Weeks,Harter JCP90 pdf p.7

Cartesian coordination at Carbon atom vertices

Cartesian coordination at Carbon atom vertices



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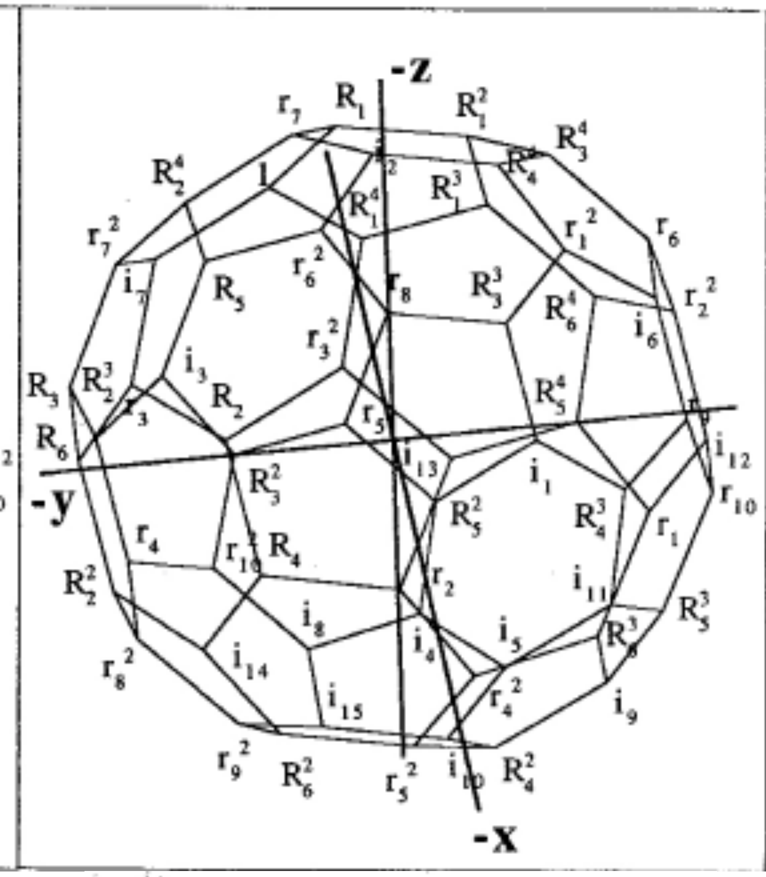

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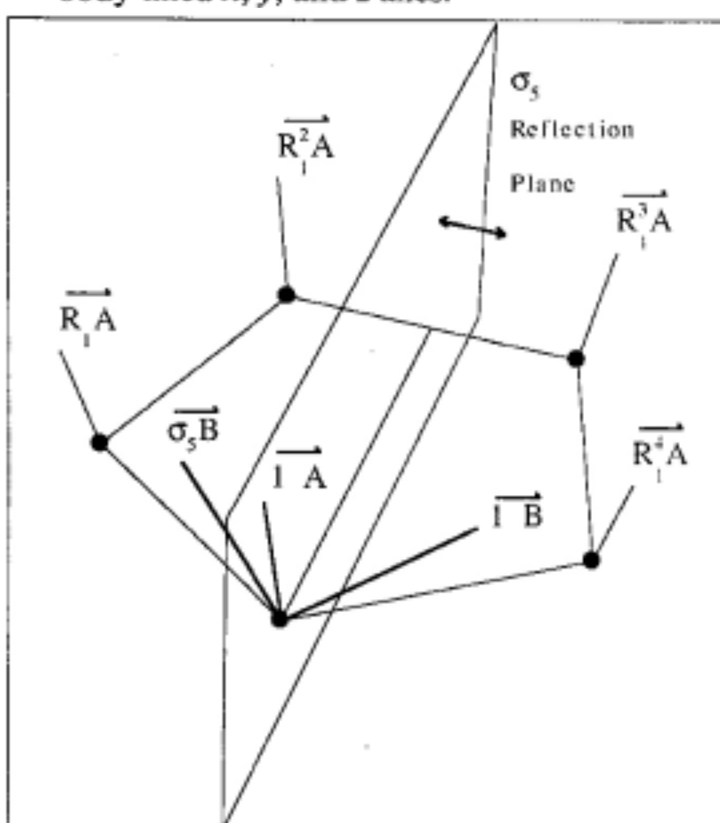

Fig. 7 *Orthonormal triad of coordinate axes relative to radial A-axis at pentagon vertex*

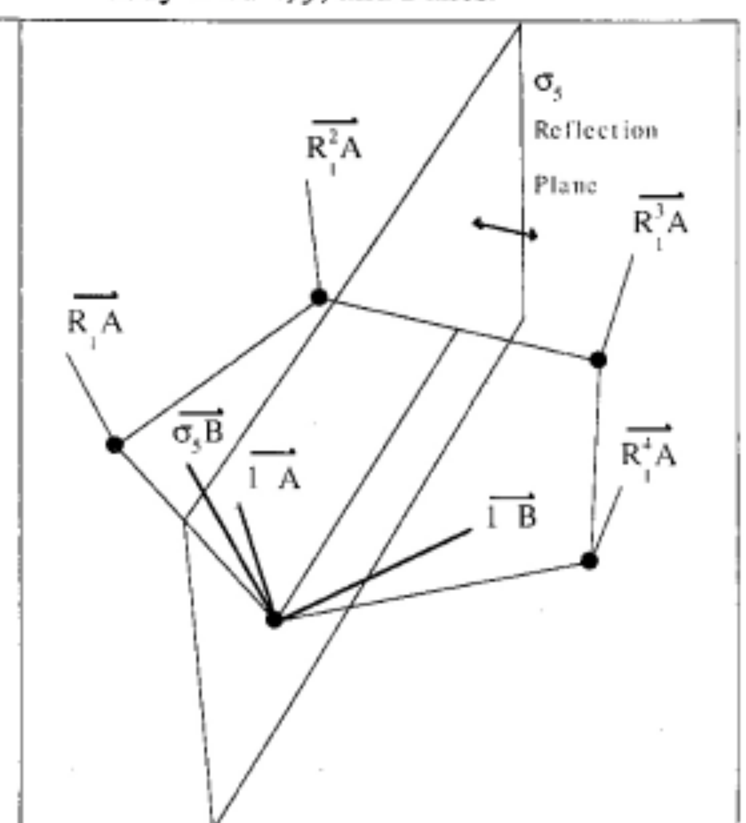

Fig. 7 *Orthonormal triad of coordinate axes relative to radial A-axis at pentagon vertex*

FIG. 7. Orientation and labeling of the symmetrically defined coordinate axes located at the unit vertex. The σ_5 reflection plane used to reflect $1B$ into $\sigma_5 B$ is illustrated.

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Cartesian coordination at Carbon atom vertices

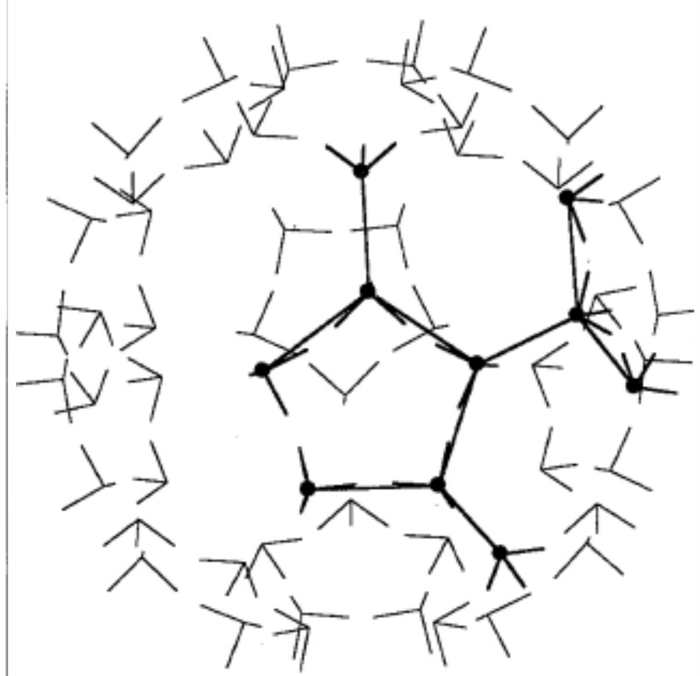
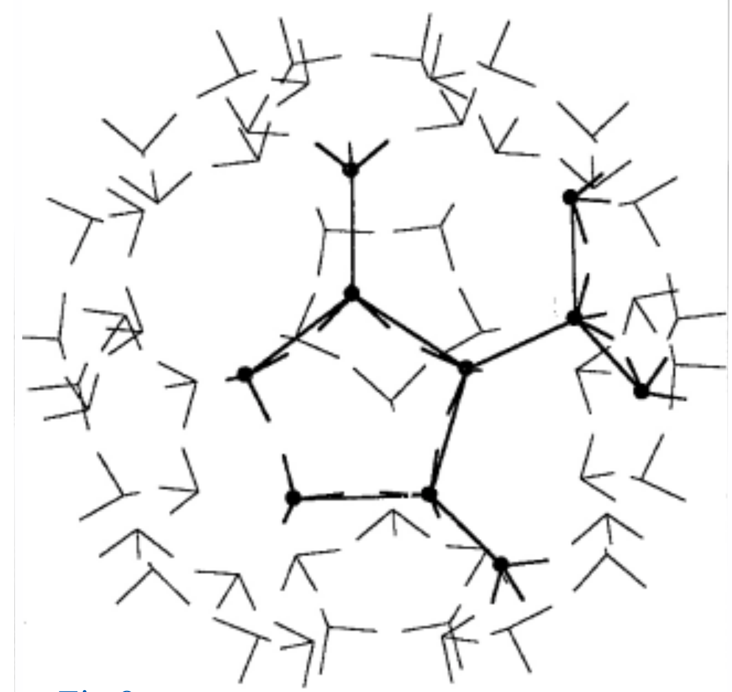


Fig.8
60 orthonormal triads of coordinate axes. Unit cell used to define force matrix has thicker lines

Cartesian coordination at Carbon atom vertices



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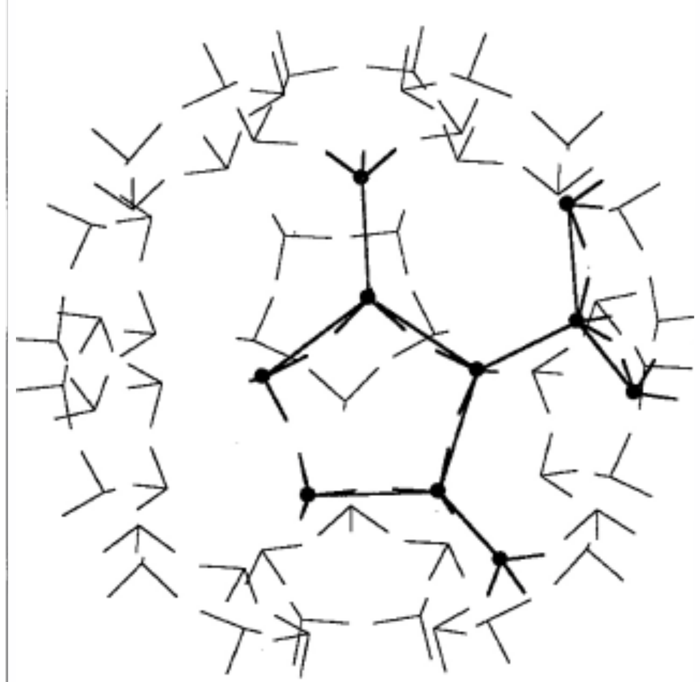
Cartesian coordination at Carbon atom vertices



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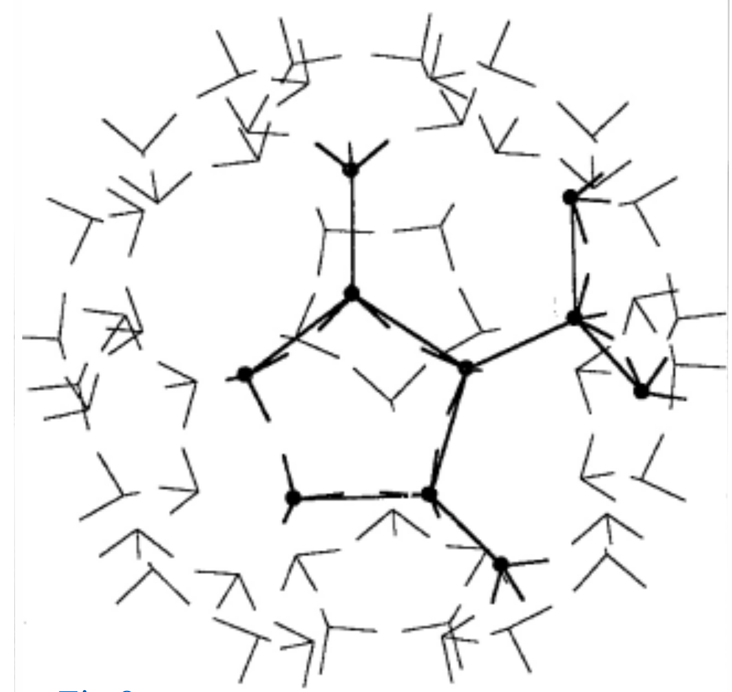

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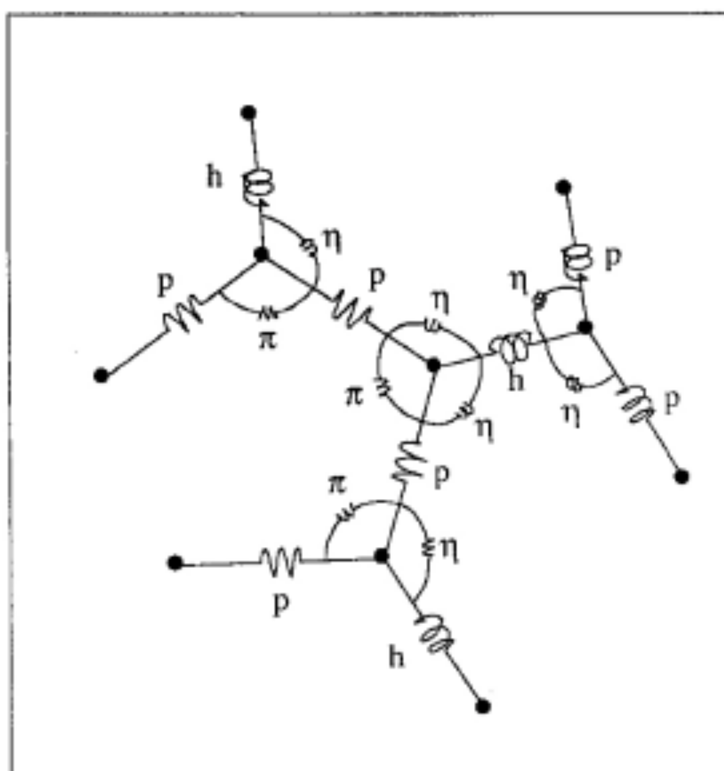

Fig.9
Springs of the dark-lined unit cell in Fig. 8 involve single-bond parameters (p,π) and double-bond parameters (h,η).

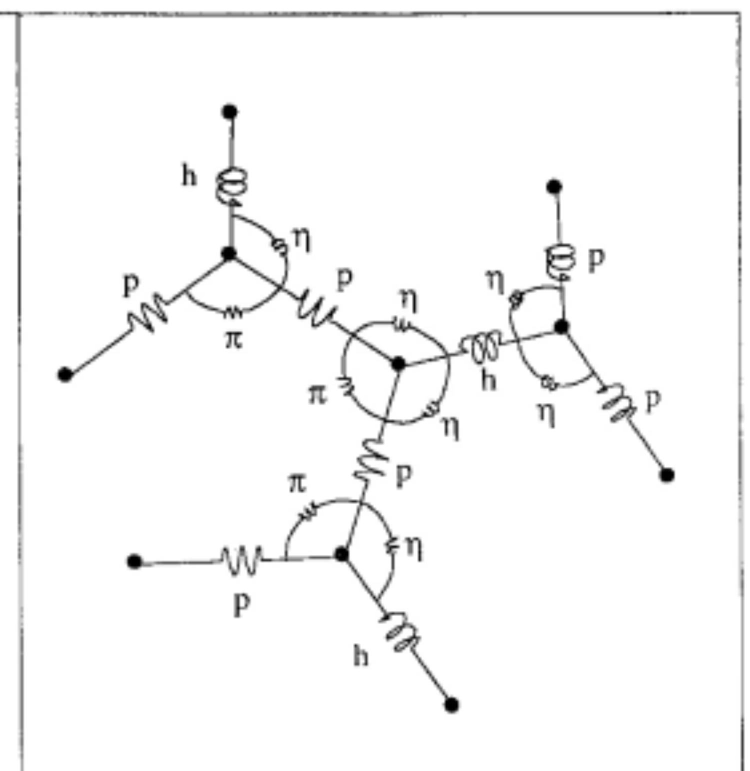

Fig.9
Springs of the dark-lined unit cell in Fig. 8 involve single-bond parameters (p,π) and double-bond parameters (h,η).

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Icosahedral subgroup $I \subset I_h$ isomorphic to even-permutation group $A_5 \subset S_5$

C_{60} Cartesian coordination at Carbon atom vertices

➡ Force vectors and matrices

I_h characters $\chi^{(\alpha)}$ and irreps $d^{(A)} \uparrow D^{(\alpha)}$ and $D^{(\alpha)} \downarrow d^{(A)}$ correlations.   Icosahedral irreps $D^{(\alpha)}$

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Tensor centrifugal effects for high-J rotation of C_{60} Rotational-Energy-Surfaces (RES)

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Comparing SF_6 with $^{13}C_{60}$ and CF_4 and OsO_4 with $^{12}C_{60}$…

Total nuclear spin-weights of each $^{13}C_{60}$ symmetry species

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$^{13}C^{12}C_{59}$ isotopomers and their RES

Some history of C_{60} discoveries

Force vectors and matrices

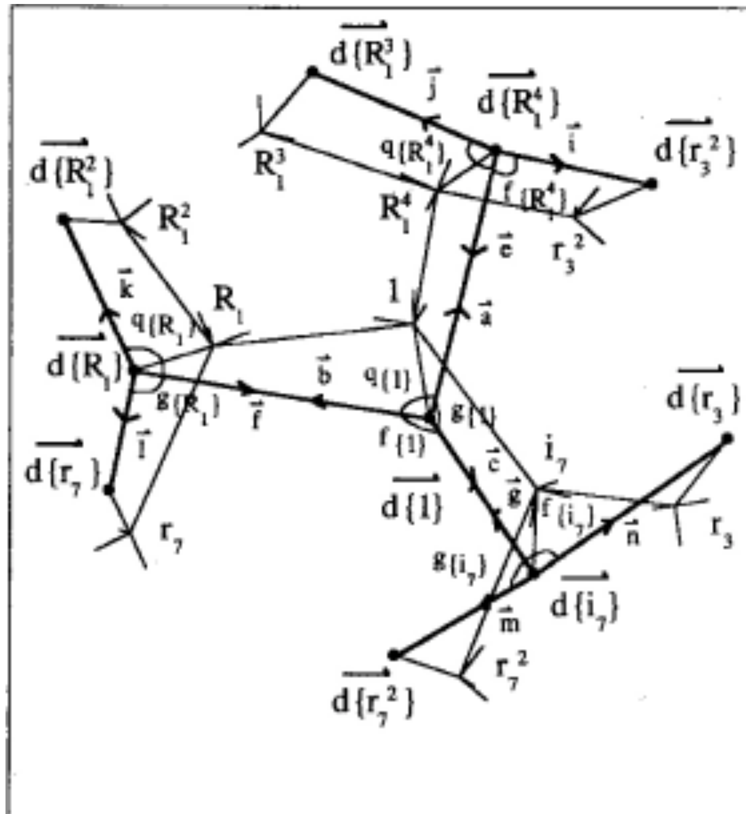
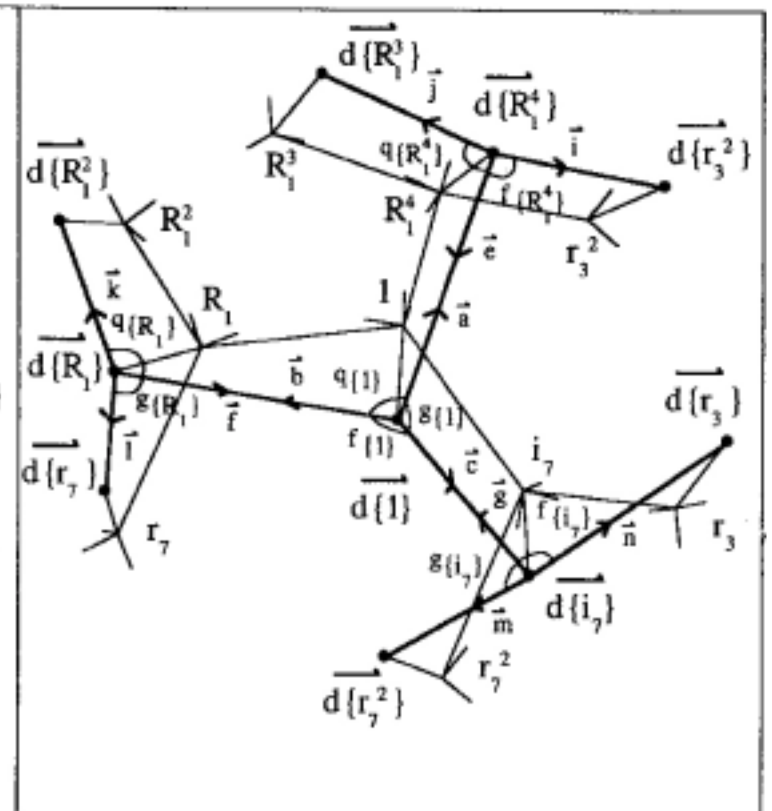


Fig.10
3D view of distorted unit cell shows vectors and angles that determine potential within a group operator defined coordinate system.



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3D view of distorted unit cell shows vectors and angles that determine potential within a group operator defined coordinate system.

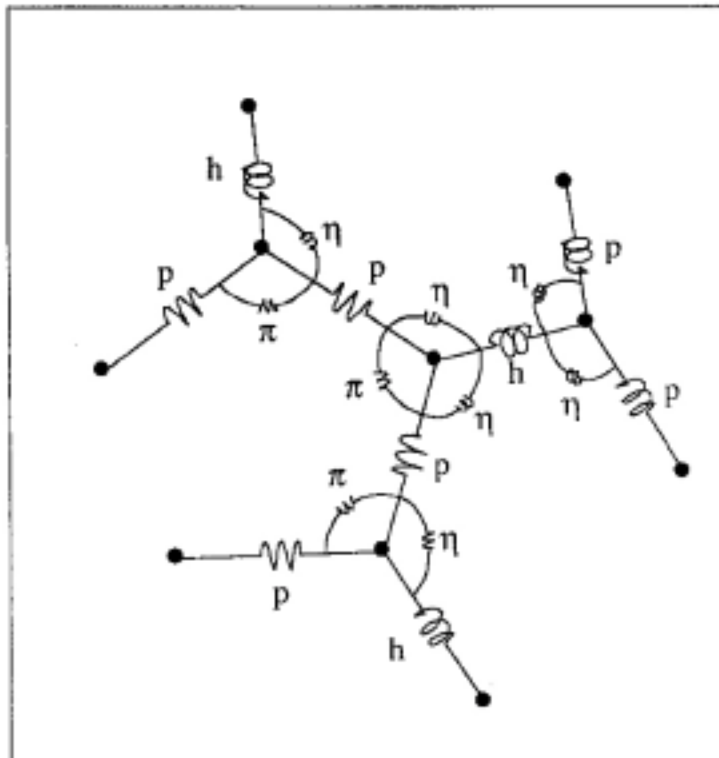

Fig.9
Springs of the dark-lined unit cell in Fig. 8 involve single-bond parameters (p,π) and double-bond parameters (h,η).

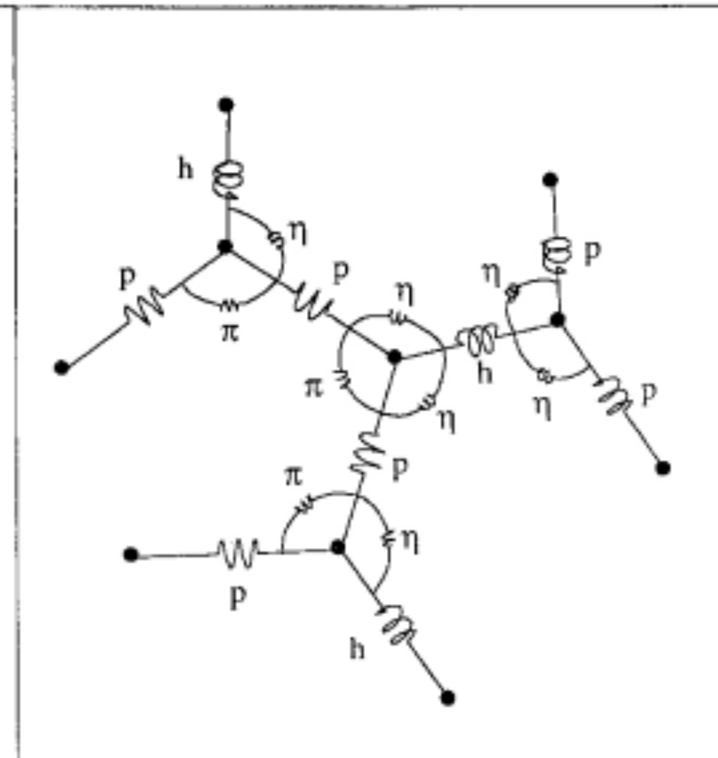

Fig.9
Springs of the dark-lined unit cell in Fig. 8 involve single-bond parameters (p,π) and double-bond parameters (h,η).

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Force vectors and matrices

TABLE I. Nonzero elements of the $\langle 1A \vert$ and $\langle 1B \vert$ rows of the initial force matrix as a function of spring constants p, h, π, and η.

$\langle 1A \vert \mathbf{K} \vert 1A \rangle$	$= (0.081426)p + (0.040713)h + (0.462764)\pi + (1.46566)\eta$	$\langle 1A \vert \mathbf{K} \vert r_3A \rangle$	$= (0)p + (0)h + (0)\pi + (0.122138)\eta$
$\langle 1A \vert \mathbf{K} \vert 1B \rangle$	$= -(0.157533)p + (0.139741)h - (0.895307)\pi + (1.09754)\eta$	$\langle 1A \vert \mathbf{K} \vert r_3B \rangle$	$= (0)p + (0)h + (0)\pi + (0.085289)\eta$
$\langle 1A \vert \mathbf{K} \vert \sigma_5B \rangle$	$= -(0.157533)p + (0.139741)h - (0.895307)\pi + (1.09754)\eta$	$\langle 1A \vert \mathbf{K} \vert \rho_r^3B \rangle$	$= (0)p + (0)h + (0)\pi + (0.316143)\eta$
$\langle 1A \vert \mathbf{K} \vert i_7A \rangle$	$= (0)p + (0.040713)h + (0)\pi - (0.977107)\eta$	$\langle 1A \vert \mathbf{K} \vert r_3^2A \rangle$	$= (0)p + (0)h + (0)\pi + (0.122138)\eta$
$\langle 1A \vert \mathbf{K} \vert i_7B \rangle$	$= (0)p + (0.139741)h + (0)\pi - (0.294679)\eta$	$\langle 1A \vert \mathbf{K} \vert r_3^2B \rangle$	$= (0)p + (0)h + (0)\pi - (0.248647)\eta$
$\langle 1A \vert \mathbf{K} \vert \sigma_{11}B \rangle$	$= (0)p + (0.139741)h + (0)\pi - (0.294679)\eta$	$\langle 1A \vert \mathbf{K} \vert \rho_5^2B$	$= (0)p + (0)h + (0)\pi + (0.213062)\eta$
$\langle 1A \vert \mathbf{K} \vert R_1^4A \rangle$	$= (0.040713)p + (0)h - (0.308510)\pi - (0.488553)\eta$	$\langle 1A \vert \mathbf{K} \vert R_1^3A \rangle$	$= (0)p + (0)h + (0.077127)\pi + (0)\eta$
$\langle 1A \vert \mathbf{K} \vert R_1^4B \rangle$	$= (0.036660)p + (0)h + (0.827726)\pi - (1.16149)\eta$	$\langle 1A \vert \mathbf{K} \vert R_1^3B \rangle$	$= (0)p + (0)h - (0.264645)\pi + (0)\eta$
$\langle 1A \vert \mathbf{K} \vert \sigma_4B \rangle$	$= -(0.194194)p + (0)h + (0.366017)\pi - (0.007219)\eta$	$\langle 1A \vert \mathbf{K} \vert \sigma_8B \rangle$	$= (0)p + (0)h - (0.033791)\pi + (0)\eta$
$\langle 1A \vert \mathbf{K} \vert R_1A \rangle$	$= (0.040713)p + (0)h - (0.308510)\pi - (0.488553)\eta$	$\langle 1A \vert \mathbf{K} \vert R_1^2A \rangle$	$= (0)p + (0)h + (0.077127)\pi + (0)\eta$
$\langle 1A \vert \mathbf{K} \vert R_1B \rangle$	$= -(0.194194)p + (0)h + (0.366017)\pi - (0.007219)\eta$	$\langle 1A \vert \mathbf{K} \vert R_1^2B \rangle$	$= (0)p + (0)h - (0.33791)\pi + (0)\eta$
$\langle 1A \vert \mathbf{K} \vert \sigma_{10}B \rangle$	$= (0.036660)p + (0)h + (0.827726)\pi - (1.16149)\eta$	$\langle 1A \vert \mathbf{K} \vert \sigma_{15}B \rangle$	$= (0)p + (0)h - (0.264645)\pi + (0)\eta$
$\langle 1A \vert \mathbf{K} \vert r_7^2A \rangle$	$= (0)p + (0)h + (0)\pi + (0.122138)\eta$	$\langle 1A \vert \mathbf{K} \vert r_7A \rangle$	$= (0)p + (0)h + (0)\pi + (0.122138)\eta$
$\langle 1A \vert \mathbf{K} \vert r_7^2B \rangle$	$= (0)p + (0)h + (0)\pi + (0.316143)\eta$	$\langle 1A \vert \mathbf{K} \vert r_7B \rangle$	$= (0)p + (0)h + (0)\pi + (0.213062)\eta$
$\langle 1A \vert \mathbf{K} \vert \rho_5^3B \rangle$	$= (0)p + (0)h + (0)\pi + (0.085289)\eta$	$\langle 1A \vert \mathbf{K} \vert \rho_4^2B \rangle$	$= (0)p + (0)h + (0)\pi - (0.248647)\eta$
$\langle 1B \vert \mathbf{K} \vert 1A \rangle$	$= -(0.157533)p + (0.139741)h - (0.895307)\pi + (1.09754)\eta$	$\langle 1B \vert \mathbf{K} \vert r_3A \rangle$	$= (0)p + (0)h + (0)\pi - (0.248646)\eta$
$\langle 1B \vert \mathbf{K} \vert 1B \rangle$	$= (0.959287)p + (0.479644)h + (2.07763)\pi + (4.26717)\eta$	$\langle 1B \vert \mathbf{K} \vert r_3B \rangle$	$= (0)p + (0)h + (0)\pi - (0.173629)\eta$
$\langle 1B \vert \mathbf{K} \vert \sigma_5B \rangle$	$= -(0.349730)p + (0.479644)h + (1.38665)\pi - (1.84158)\eta$	$\langle 1B \vert \mathbf{K} \vert \rho_4^3B \rangle$	$= (0)p + (0)h + (0)\pi - (0.643597)\eta$
$\langle 1B \vert \mathbf{K} \vert i_7A \rangle$	$= (0)p + (0.139741)h + (0)\pi - (0.294679)\eta$	$\langle 1B \vert \mathbf{K} \vert r_3^2A \rangle$	$= (0)p + (0)h + (0)\pi + (0.085289)\eta$
$\langle 1B \vert \mathbf{K} \vert i_7B \rangle$	$= (0)p + (0.479644)h + (0)\pi + (2.72462)\eta$	$\langle 1B \vert \mathbf{K} \vert r_3^2B \rangle$	$= (0)p + (0)h + (0)\pi - (0.173629)\eta$
$\langle 1B \vert \mathbf{K} \vert \sigma_{11}B \rangle$	$= (0)p + (0.479644)h + (0)\pi - (2.511145)\eta$	$\langle 1B \vert \mathbf{K} \vert \rho_5^2B \rangle$	$= (0)p + (0)h + (0)\pi + (0.148780)\eta$
$\langle 1B \vert \mathbf{K} \vert R_1^4A \rangle$	$= -(0.194194)p + (0)h + (0.366017)\pi - (0.007219)\eta$	$\langle 1B \vert \mathbf{K} \vert R_1^3A \rangle$	$= (0)p + (0)h - (0.033791)\pi + (0)\eta$
$\langle 1B \vert \mathbf{K} \vert R_1^4B \rangle$	$= -(0.174865)p + (0)h - (1.15476)\pi + (0.053294)\eta$	$\langle 1B \vert \mathbf{K} \vert R_1^3B \rangle$	$= (0)p + (0)h + (0.115945)\pi + (0)\eta$
$\langle 1B \vert \mathbf{K} \vert \sigma_4B \rangle$	$= (0.926276)p + (0)h - (0.261498)\pi + (0.228144)\eta$	$\langle 1B \vert \mathbf{K} \vert \sigma_8B \rangle$	$= (0)p + (0)h + (0.014804)\pi + (0)\eta$
$\langle 1B \vert \mathbf{K} \vert R_1A \rangle$	$= (0.036660)p + (0)h + (0.827726)\pi - (1.16149)\eta$	$\langle 1B \vert \mathbf{K} \vert R_1^2A \rangle$	$= (0)p + (0)h - (0.264645)\pi + (0)\eta$
$\langle 1B \vert \mathbf{K} \vert R_1B \rangle$	$= -(0.174865)p + (0)h - (1.15476)\pi + (0.053294)\eta$	$\langle 1B \vert \mathbf{K} \vert R_1^2B \rangle$	$= (0)p + (0)h + (0.115945)\pi + (0)\eta$
$\langle 1B \vert \mathbf{K} \vert \sigma_{10}B \rangle$	$= (0.033011)p + 0)h - (2.04803)\pi - (2.73959)\eta$	$\langle 1B \vert \mathbf{K} \vert \sigma_{15}B \rangle$	$= (0)p + (0)h + (0.908068)\pi + (0)\eta$
$\langle 1B \vert \mathbf{K} \vert r_7^2A \rangle$	$= (0)p + (0)h + (0)\pi + (0.213062)\eta$	$\langle 1B \vert \mathbf{K} \vert r_7A \rangle$	$= (0)p + (0)h + (0)\pi + (0.316143)\eta$
$\langle 1B \vert \mathbf{K} \vert r_7^2B \rangle$	$= (0)p + (0)h + (0)\pi + (0.551490)\eta$	$\langle 1B \vert \mathbf{K} \vert r_7B \rangle$	$= (0)p + (0)h + (0)\pi + (0.551490)\eta$
$\langle 1B \vert \mathbf{K} \vert \rho_5^3B \rangle$	$= (0)p + (0)h + (0)\pi + (0.148780)\eta$	$\langle 1B \vert \mathbf{K} \vert \rho_4^2B \rangle$	$= (0)p + (0)h + (0)\pi - (0.643597)\eta$

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AMOP reference links on pages 2-4

5.08.18 class 29: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

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Icosahedral I_h characters $\chi^{(\alpha)}$ and irrep $d^{(A)}\uparrow D^{(\alpha)}$ and $D^{(\alpha)}\downarrow d^{(A)}$ correlations

$I_h \supset I$	0° $\mathbf{1}_1$	72° $\mathbf{R}^{1,4}_{12}$	144° $\mathbf{R}^{2,3}_{12}$	120° $\mathbf{r}^{2,3}_{20}$	180° $\mathbf{i}^{1}_{15}$	$\mathbf{I}_1$	72°**I** $\rho^{1,4}_{12}$	144°**I** $\rho^{2,3}_{12}$	120°**I** $\eta^{2,3}_{20}$	180°**I** σ^{1}_{15}
A_g	1	1	1	1	1	1	1	1	1	1
T_{1g}	3	G_+	G_-	·	-1	3	G_+	G_-	·	-1
T_{3g}	3	G_-	G_+	·	-1	3	G_-	G_+	·	-1
G_g	4	-1	-1	1	·	4	-1	-1	1	·
H_g	5	·	·	-1	1	5	·	·	-1	1
A_u	1	1	1	1	1	-1	-1	-1	-1	-1
T_{1u}	3	G_+	G_-	·	-1	-3	$-G_+$	$-G_-$	·	1
T_{3u}	3	G_-	G_+	·	-1	-3	$-G_-$	$-G_+$	·	1
G_u	4	-1	-1	1	·	-4	1	1	-1	·
H_u	5	·	·	-1	1	-5	·	·	1	-1

$$G_{\pm} = \frac{1 \pm \sqrt{5}}{2}$$

S_5 Characters

S_5	1^5	21^3	$2^2 1$	31^2	32	41	5
□□□□□	1	1	1	1	1	1	1
□□□□ □	4	2	0	1	−1	0	−1
□□□ □□	5	−1	1	−1	−1	1	0
□□□ □ □	6	0	−2	0	0	0	1
□□ □□ □	5	1	1	−1	1	−1	0
□□ □ □ □	4	−2	0	1	1	0	−1
□ □ □ □ □	1	−1	1	1	−1	−1	1

Odd=red Even=green

I-Characters Harter,Weeks JCP90 pdf p.15

Weeks,Harter JCP90 pdf p.26

IC_3C_5Correlations Harter,Weeks JCP90 pdf p.9

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A_g	1	1	1	1	1	1	1	1	1	1
T_{1g}	3	G_+	G_-	·	-1	3	G_+	G_-	·	-1
T_{3g}	3	G_-	G_+	·	-1	3	G_-	G_+	·	-1
G_g	4	-1	-1	1	·	4	-1	-1	1	·
H_g	5	·	·	-1	1	5	·	·	-1	1
A_u	1	1	1	1	1	-1	-1	-1	-1	-1
T_{1u}	3	G_+	G_-	·	-1	-3	$-G_+$	$-G_-$	·	1
T_{3u}	3	G_-	G_+	·	-1	-3	$-G_-$	$-G_+$	·	1
G_u	4	-1	-1	1	·	-4	1	1	-1	·
H_u	5	·	·	-1	1	-5	·	·	1	-1

$$G_\pm = \frac{1 \pm \sqrt{5}}{2}$$

$I_h \supset C_v$	A	B
A_g	1	·
T_{1g}	1	2
T_{3g}	1	2
G_g	2	2
H_g	3	2
A_u	·	1
T_{1u}	2	1
T_{3u}	2	1
G_u	2	2
H_u	2	3

$I_h \supset C_{2h}$	A_1	A_2	B_1	B_2
A_g	1	·	·	·
T_{1g}	·	1	1	1
T_{3g}	·	1	1	1
G_g	1	1	1	1
H_g	2	1	1	1
A_u	·	·	·	1
T_{1u}	1	1	1	·
T_{3u}	1	1	1	·
G_u	1	1	1	1
H_u	1	1	1	2

$I_h \supset C_{5v}$	A_1	A_2	E_1	E_2
A_g	1	·	·	·
T_{1g}	·	1	1	·
T_{3g}	·	1	·	1
G_g	·	·	1	1
H_g	1	·	1	1
A_u	·	1	·	·
T_{1u}	1	·	1	·
T_{3u}	1	·	·	1
G_u	·	·	1	1
H_u	·	1	1	1

I-Characters Harter,Weeks JCP90 pdf p.15

IC_3C_5Correlations Harter,Weeks JCP90 pdf p.9

Icosahedral I_h characters $\chi^{(\alpha)}$ and irrep $d^{(A)}\uparrow D^{(\alpha)}$ and $D^{(\alpha)}\downarrow d^{(A)}$ correlations

$I_h \supset I$	0° $\mathbf{1}_1$	72° $\mathbf{R}^{1,4}_{12}$	144° $\mathbf{R}^{2,3}_{12}$	120° $\mathbf{r}^{2,3}_{20}$	180° $\mathbf{i}^{1}_{15}$	$\mathbf{I}_1$	72°$\mathbf{I}$ $\rho^{1,4}_{12}$	144°$\mathbf{I}$ $\rho^{2,3}_{12}$	120°$\mathbf{I}$ $\eta^{2,3}_{20}$	180°$\mathbf{I}$ σ^{1}_{15}
A_g	1	1	1	1	1	1	1	1	1	1
T_{1g}	3	G_+	G_-	·	-1	3	G_+	G_-	·	-1
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H_g	5	·	·	-1	1	5	·	·	-1	1
A_u	1	1	1	1	1	-1	-1	-1	-1	-1
T_{1u}	3	G_+	G_-	·	-1	-3	$-G_+$	$-G_-$	·	1
T_{3u}	3	G_-	G_+	·	-1	-3	$-G_-$	$-G_+$	·	1
G_u	4	-1	-1	1	·	-4	1	1	-1	·
H_u	5	·	·	-1	1	-5	·	·	1	-1

$$G_\pm = \frac{1 \pm \sqrt{5}}{2}$$

$I_h \supset C_v$	A	B
A_g	1	·
T_{1g}	1	2
T_{3g}	1	2
G_g	2	2
H_g	3	2
A_u	·	1
T_{1u}	2	1
T_{3u}	2	1
G_u	2	2
H_u	2	3

Rotational correlations for later use:

$I \supset C_2$	0_2	1_2
A	1	·
T_1	1	2
T_3	1	2
G	2	2
H	3	2

$I \supset C_5$	0_5	1_5	2_5	3_5	4_5
A	1	·	·	·	·
T_1	1	1	·	·	1
T_3	1	·	1	1	·
G	·	1	1	1	1
H	1	1	1	1	1

$I \supset C_3$	0_3	1_3	2_3
A	1	·	·
T_1	1	1	1
T_3	1	1	1
G	2	1	1
H	1	2	2

$I_h \supset C_{2h}$	A_1	A_2	B_1	B_2
A_g	1	·	·	·
T_{1g}	·	1	1	1
T_{3g}	·	1	1	1
G_g	1	1	1	1
H_g	2	1	1	1
A_u	·	·	·	1
T_{1u}	1	1	1	·
T_{3u}	1	1	1	·
G_u	1	1	1	1
H_u	1	1	1	2

$I_h \supset C_{5v}$	A_1	A_2	E_1	E_2
A_g	1	·	·	·
T_{1g}	·	1	1	·
T_{3g}	·	1	·	1
G_g	·	·	1	1
H_g	1	·	1	1
A_u	·	1	·	·
T_{1u}	1	·	1	·
T_{3u}	1	·	·	1
G_u	·	·	1	1
H_u	·	1	1	1

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Icosahedral irreps $D^{(\alpha)}$

Icosahedral Generator Irreps

$$D^{A}(r_1)=\begin{bmatrix}1\end{bmatrix}$$

$$D^{T_1}(r_1)=\begin{bmatrix}\Omega & -N & -V\\ N & -\Sigma & T\\ -V & -T & A\end{bmatrix}$$

$$D^{T_3}(r_1)=\begin{bmatrix}-\Omega & Y & G\\ -Y & -\Sigma & D\\ G & -D & Z\end{bmatrix}$$

$$D^{G}(r_1)=\begin{bmatrix}X & F & \Sigma & D\\ -F & -C & T & -S\\ \Sigma & -T & -I & -L\\ -D & -S & L & Q\end{bmatrix}$$

$$D^{H}(r_1)=\begin{bmatrix}-\Delta & E & -R & P & -K\\ E & -J & -H & \Gamma & W\\ R & H & -\Sigma & -M & .\\ P & \Gamma & M & O & -B\\ K & -W & . & B & -\Sigma\end{bmatrix}$$

$$D^{H}(i_{11})=\begin{bmatrix}-\Delta & U & . & -U & .\\ U & \Lambda & . & \Gamma & .\\ . & . & -\Omega & . & -\Psi\\ -U & \Gamma & . & \Lambda & .\\ . & . & -\Psi & . & \Omega\end{bmatrix}$$

$$D^{G}(i_{11})=\begin{bmatrix}. & . & -1 & .\\ . & \Psi & . & -\Omega\\ -1 & . & . & .\\ . & -\Omega & . & -\Psi\end{bmatrix}$$

$$D^{T_3}(i_{11})=\begin{bmatrix}\Omega & . & -\Psi\\ . & -1 & .\\ -\Psi & . & -\Omega\end{bmatrix}$$

$$D^{T_1}(i_{11})=\begin{bmatrix}-\Omega & . & -\Psi\\ . & -1 & .\\ -\Psi & . & \Omega\end{bmatrix}$$

$$D^{A}(i_{11})=\begin{bmatrix}1\end{bmatrix}$$

$A=\left(\frac{7-4G^+}{10}\right)$	$I=\left(\frac{-G^-}{2}\right)$	$Q=\left(\frac{1+3G^+}{10}\right)$	$Y=\left(\frac{2+G^+}{5}\right)^{\frac{1}{2}}$
$B=\left(\frac{7-4G^+}{100}\right)^{\frac{1}{2}}$	$J=\left(\frac{-3+4G^+}{10}\right)$	$R=\left(\frac{3G^+}{5\sqrt{5}}\right)^{\frac{1}{2}}$	$Z=\left(\frac{3+4G^+}{10}\right)$
$C=\left(\frac{-4+3G^+}{10}\right)$	$K=\left(\frac{-3G^-}{5\sqrt{5}}\right)^{\frac{1}{2}}$	$S=\left(\frac{3}{2\sqrt{5}}\right)$	$\Omega=\frac{1}{\sqrt{5}}$ $\Delta=\frac{1}{5}$
$D=\left(\frac{7-4G^+}{20}\right)^{\frac{1}{2}}$	$L=\left(\frac{2+G^+}{20}\right)^{\frac{1}{2}}$	$T=\left(\frac{3+4G^+}{20}\right)^{\frac{1}{2}}$	$\Psi=\frac{2}{\sqrt{5}}$ $\Sigma=\frac{1}{2}$
$E=\left(\frac{-\sqrt{3}G^-}{5}\right)$	$M=\left(\frac{-4G^-}{5\sqrt{5}}\right)^{\frac{1}{2}}$	$U=\left(\frac{\sqrt{12}}{5}\right)$	$\Gamma=\frac{2}{5}$ $\Lambda=\frac{3}{5}$
$F=\left(\frac{3-G^+}{20}\right)^{\frac{1}{2}}$	$N=\left(\frac{3-G^+}{5}\right)^{\frac{1}{2}}$	$V=\left(\frac{2+G^+}{5}\right)$	$G^{\pm}=\frac{1\pm\sqrt{5}}{2}$
$G=\left(\frac{3-G^+}{5}\right)$	$O=\left(\frac{-1+4G^+}{10}\right)$	$W=\left(\frac{4G^+}{5\sqrt{5}}\right)^{\frac{1}{2}}$	Irrep Key
$H=\left(\frac{3+4G^+}{100}\right)^{\frac{1}{2}}$	$P=\left(\frac{\sqrt{12}G^+}{10}\right)$	$X=\left(\frac{G^+}{2}\right)$	

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Icosahedral I_h irreps for A-orbits and B-orbits

A-orbits:

$I_h \uparrow C_v$	A	B
A_g	1	·
T_{1g}	1	2
T_{3g}	1	2
G_g	2	2
H_g	3	2
A_u	·	1
T_{1u}	2	1
T_{3u}	2	1
G_u	2	2
H_u	2	3

$$A\uparrow I_h = 1A_g \oplus 1T_{1g} \oplus 1T_{3g} \oplus 2G_g \oplus 3H_g \oplus 0A_u \oplus 2T_{1u} \oplus 2T_{3u} \oplus 2G_u \oplus 2H_u$$

(60 levels)

Icosahedral I_h irreps for A-orbits and B-orbits

A-orbits:

$I_h \uparrow C_v$	A	B
A_g	1	·
T_{1g}	1	2
T_{3g}	1	2
G_g	2	2
H_g	3	2
A_u	·	1
T_{1u}	2	1
T_{3u}	2	1
G_u	2	2
H_u	2	3

$I_h \uparrow C_1$	0_1
A_g	1
T_{1g}	3
T_{3g}	3
G_g	4
H_g	5
A_u	1
T_{1u}	3
T_{3u}	3
G_u	4
H_u	5

$$A \uparrow I_h = 1A_g \oplus 1T_{1g} \oplus 1T_{3g} \oplus 2G_g \oplus 3H_g \oplus 0A_u \oplus 2T_{1u} \oplus 2T_{3u} \oplus 2G_u \oplus 2H_u$$ *(60 levels)*

B-orbits:

$$0_1 \uparrow I_h = A_g \oplus 3T_{1g} \oplus 3T_{3g} \oplus 4G_g \oplus 5H_g \oplus 1A_u \oplus 3T_{1u} \oplus 3T_{3u} \oplus 4G_u \oplus 5H_u$$ *(120 levels)*

Icosahedral I_h irreps for A-orbits and B-orbits

A-orbits:

$I_h \uparrow C_v$	A	B
A_g	1	·
T_{1g}	1	2
T_{3g}	1	2
G_g	2	2
H_g	3	2
A_u	·	1
T_{1u}	2	1
T_{3u}	2	1
G_u	2	2
H_u	2	3

$I_h \uparrow C_1$	0_1
A_g	1
T_{1g}	3
T_{3g}	3
G_g	4
H_g	5
A_u	1
T_{1u}	3
T_{3u}	3
G_u	4
H_u	5

$$A \uparrow I_h = 1A_g \oplus 1T_{1g} \oplus 1T_{3g} \oplus 2G_g \oplus 3H_g \oplus 0A_u \oplus 2T_{1u} \oplus 2T_{3u} \oplus 2G_u \oplus 2H_u \quad \text{(60 levels)}$$

B-orbits:

$$0_1 \uparrow I_h = 1A_g \oplus 3T_{1g} \oplus 3T_{3g} \oplus 4G_g \oplus 5H_g \oplus 1A_u \oplus 3T_{1u} \oplus 3T_{3u} \oplus 4G_u \oplus 5H_u \quad \text{(120 levels)}$$

Total:

$$A + B = 2A_g \oplus 4T_{1g} \oplus 4T_{3g} \oplus 6G_g \oplus 8H_g \oplus 1A_u \oplus 5T_{1u} \oplus 5T_{3u} \oplus 6G_u \oplus 7H_u \quad \text{(180 levels)}$$

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Force matrices projected to be diagonalized

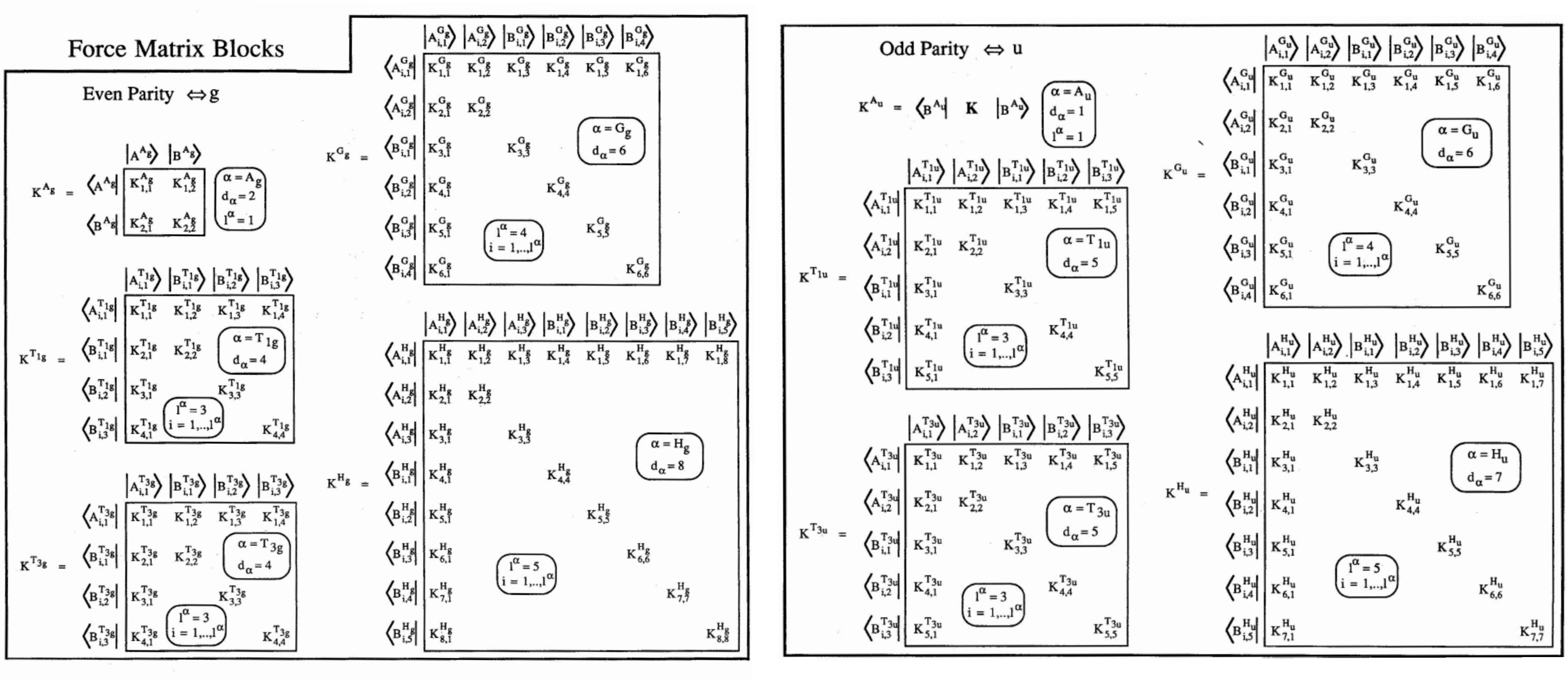

FIG. 12. Block diagonal elements of the force matrix obtained by icosahedral symmetry projection.

$$A+B=2A_g\oplus 4T_{1g}\oplus 4T_{3g}\oplus 6G_g\oplus 8H_g \quad\oplus\quad 1A_u\oplus 5T_{1u}\oplus 5T_{3u}\oplus 6G_u\oplus 7H_u$$

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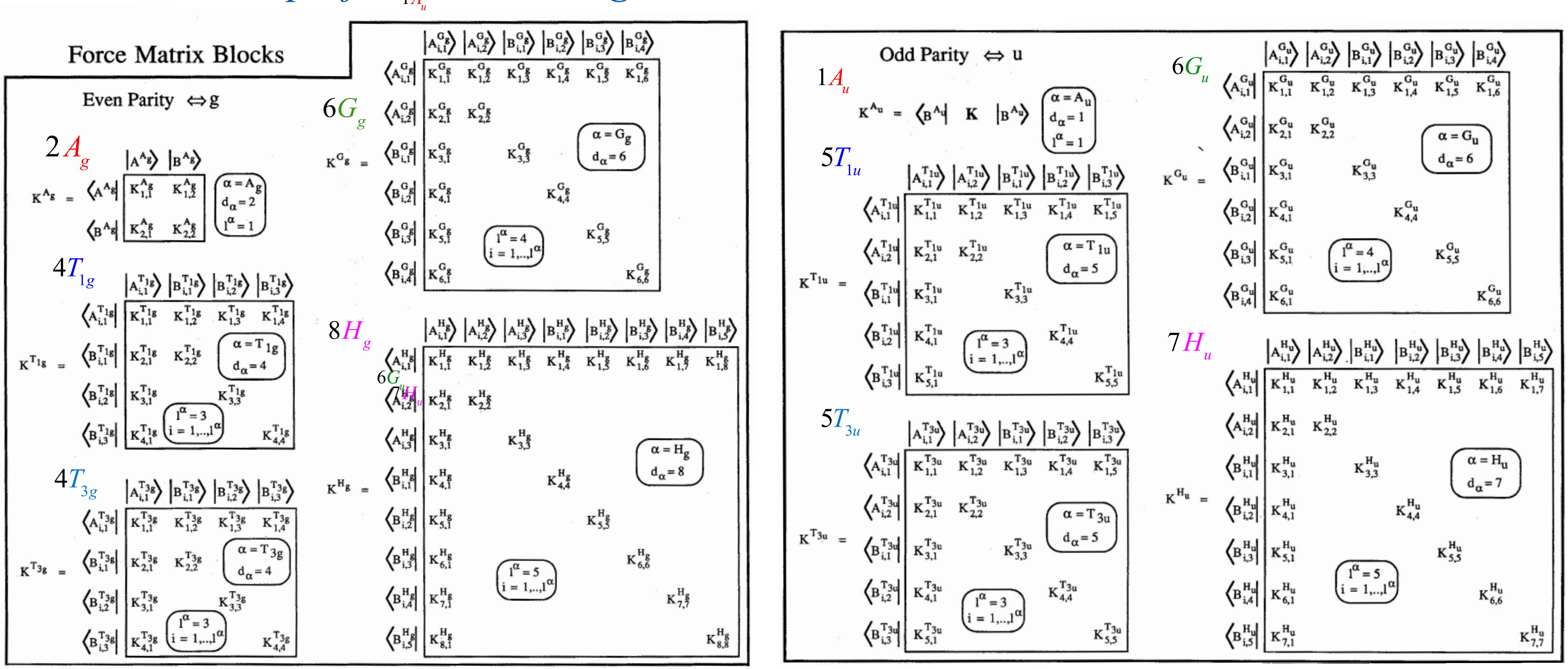
Force matrices projected to be diagonalized



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1 less T_{1g} (rotation) *1 less T_{1u} (translation)*

$$A+B=2A_g\oplus \underset{3}{\cancel{4}}T_{1g}\oplus 4T_{3g}\oplus 6G_g\oplus 8H_g \quad\oplus\quad 1A_u\oplus \underset{4}{\cancel{5}}T_{1u}\oplus 5T_{3u}\oplus 6G_u\oplus 7H_u$$

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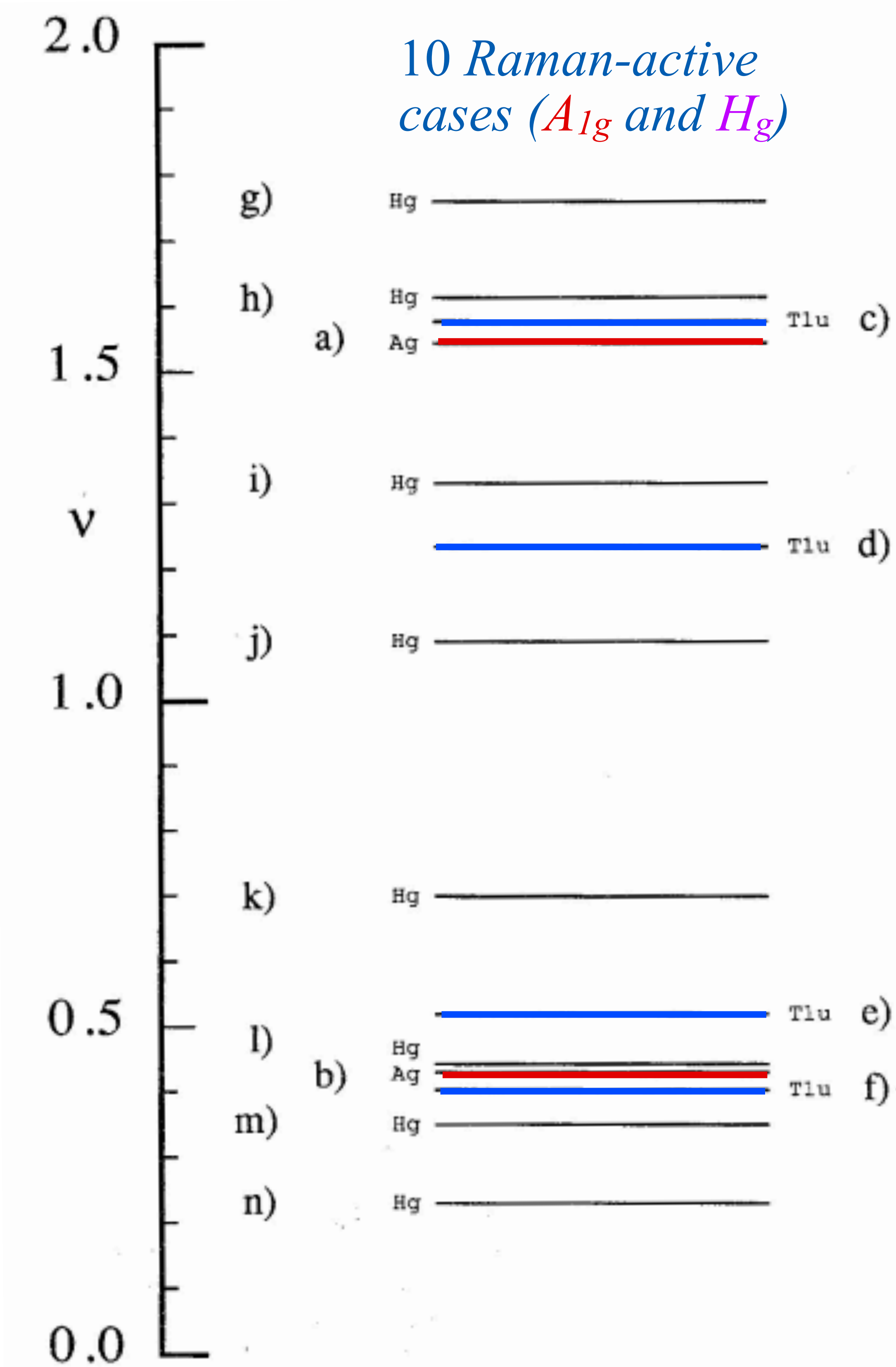

TABLE III. Symmetry labeled eigenfrequencies of buckyball for spring constants of benzene given in Eq. (5.1).

Even parity I_h group label	Even parity Frequency (1/cm)	Odd parity I_h group label	Odd parity Frequency (1/cm)
A_g	1830	A_u	1243
	510		
		T_{1u}	1868
T_{1g}	1662		1462
	1045		618
	513		478
T_{3g}	1900	T_{3u}	1954
	951		1543
	724		1122
	615		526
			358
G_g	2006		
	1813	G_u	2004
	1327		1845
	657		1086
	593		876
	433		663
			360
H_g	2085		
	1910	H_u	2086
	1575		1797
	1292		1464
	828		849
	526		569
	413		470
	274		405

2 Raman-active (A_g)

3 T_{1g} rotor-like modes

4 T_{1u} — 4 infrared-active (T_{1u})

8 Raman-active (H_g)

1 less T_{1g} (rotation)

1 less T_{1u} (translation)

$$A+B = 2A_g \oplus \cancel{4}\,3\,T_{1g} \oplus 4T_{3g} \oplus 6G_g \oplus 8H_g \quad \oplus \quad 1A_u \oplus \cancel{5}\,4\,T_{1u} \oplus 5T_{3u} \oplus 6G_u \oplus 7H_u$$

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Mode frequency variation with locked force parameters π=η versus p=h

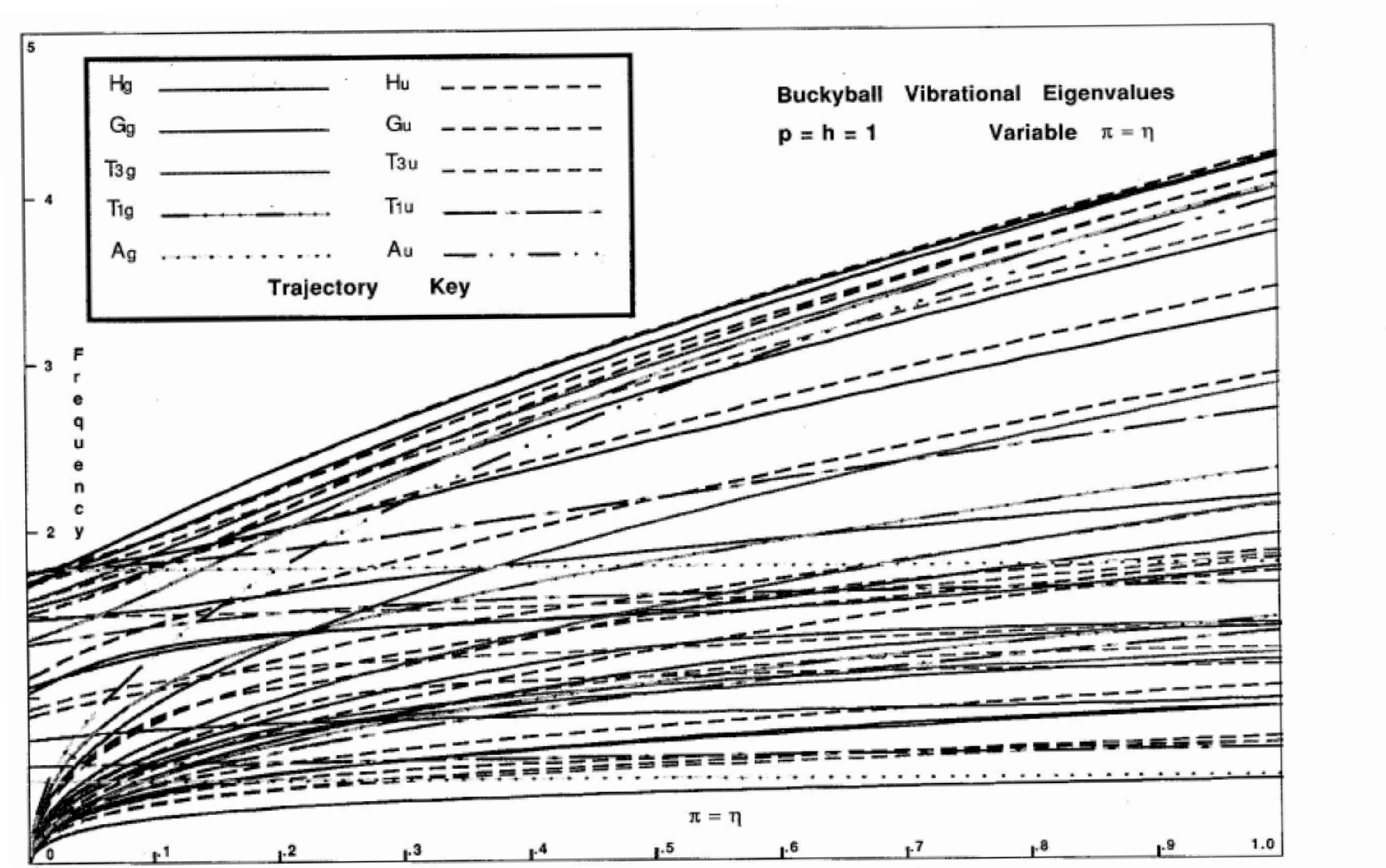
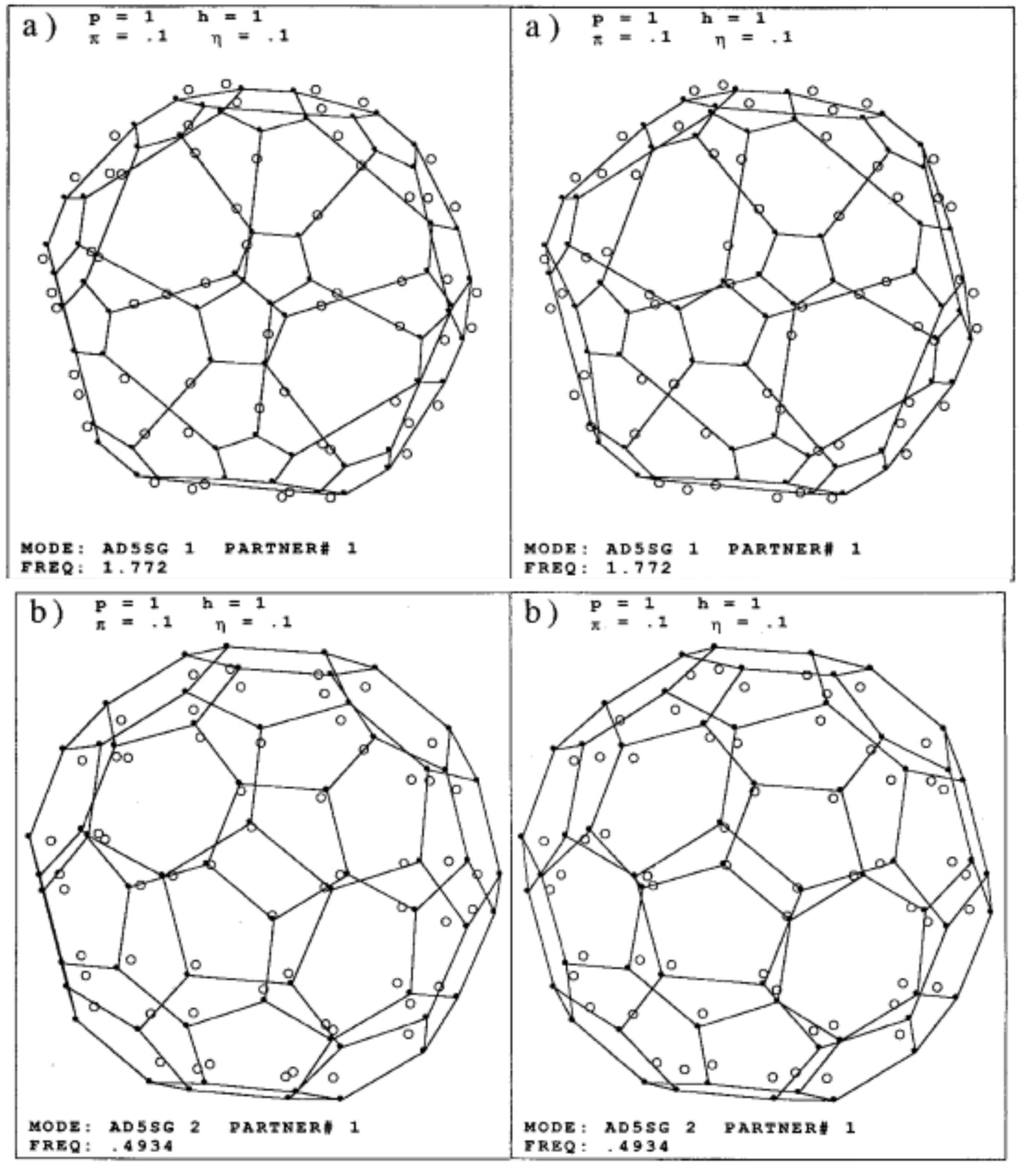
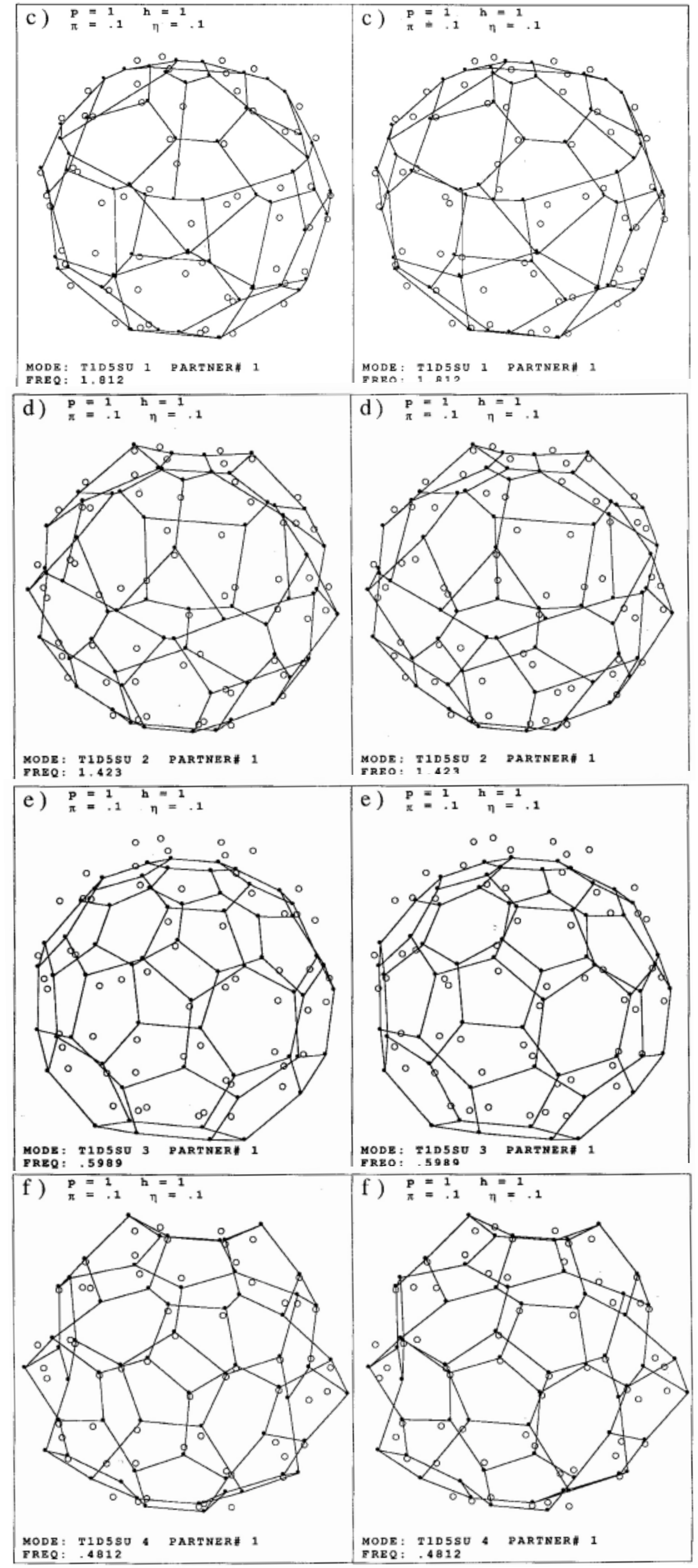


FIG. 13. Buckyball vibrational eigenvalue trajectories. Note the near degenerate avoided crossing of the lowest two T_{1u} trajectories at $\pi = \eta = 0.17$.

IR-active and most-Raman-active modes in 3D



Raman-active cases (A_{1g})



4 infrared-active cases (T_{1u})

(It is amazing how such a symmetric molecule forms polar dipoles.)

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Comparing T_{1u}-(x+iy) mode ellipticity and zeta factors ζ

Coriolis *zeta* factors:

$$\zeta^{\gamma} = \sum_{i=1}^{60} \left(|\alpha_i\rangle\langle\beta_i| - |\beta_i\rangle\langle\alpha_i| \right) \quad \text{Body-fixed Cartesian: } x=\alpha,\ \ y=\beta,\ \ z=\gamma.$$

$$\zeta^{\gamma}_{m_x,m_y} = \sum_{i=1}^{60} \left(\langle m_x|\beta_i\rangle\langle\alpha_i|m_y\rangle - \langle m_x|\alpha_i\rangle\langle\beta_i|m_y\rangle \right)$$

$$\equiv \zeta^{\gamma}_{m} = \sum_{i=1}^{60} \left(Q^{*}_{m_x,\beta_i} Q_{m_y,\alpha_i} - Q^{*}_{m_x,\alpha_i} Q_{m_y,\beta_i} \right)$$

$m = 1, 2, 3,$ or 4 indexes the T_{1u} vector modes

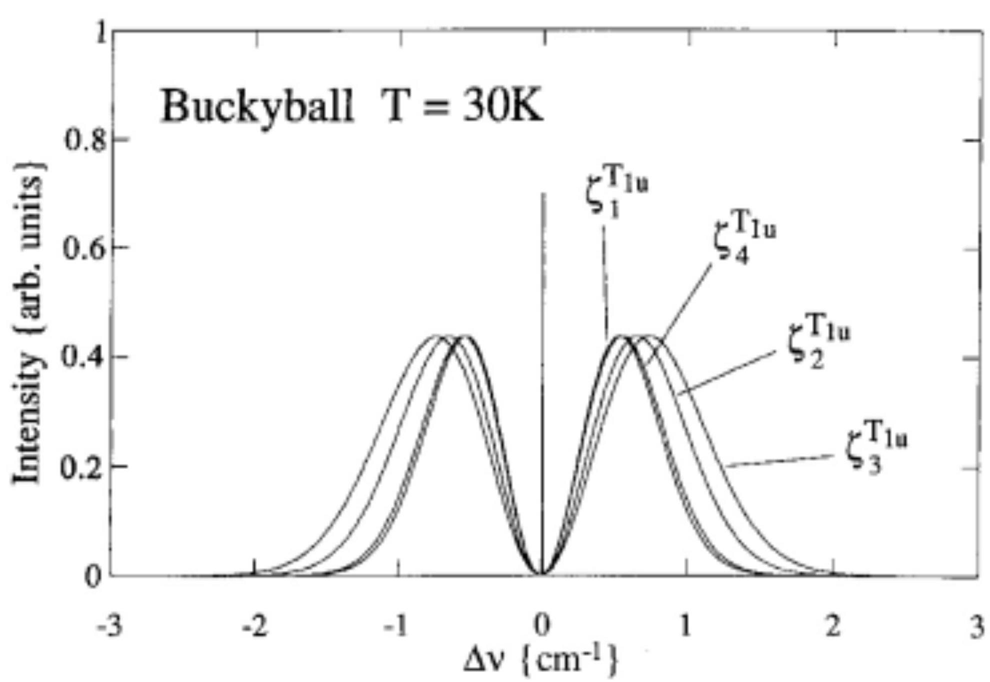
$$\zeta_1^{T_{1u}} = -0.07613$$

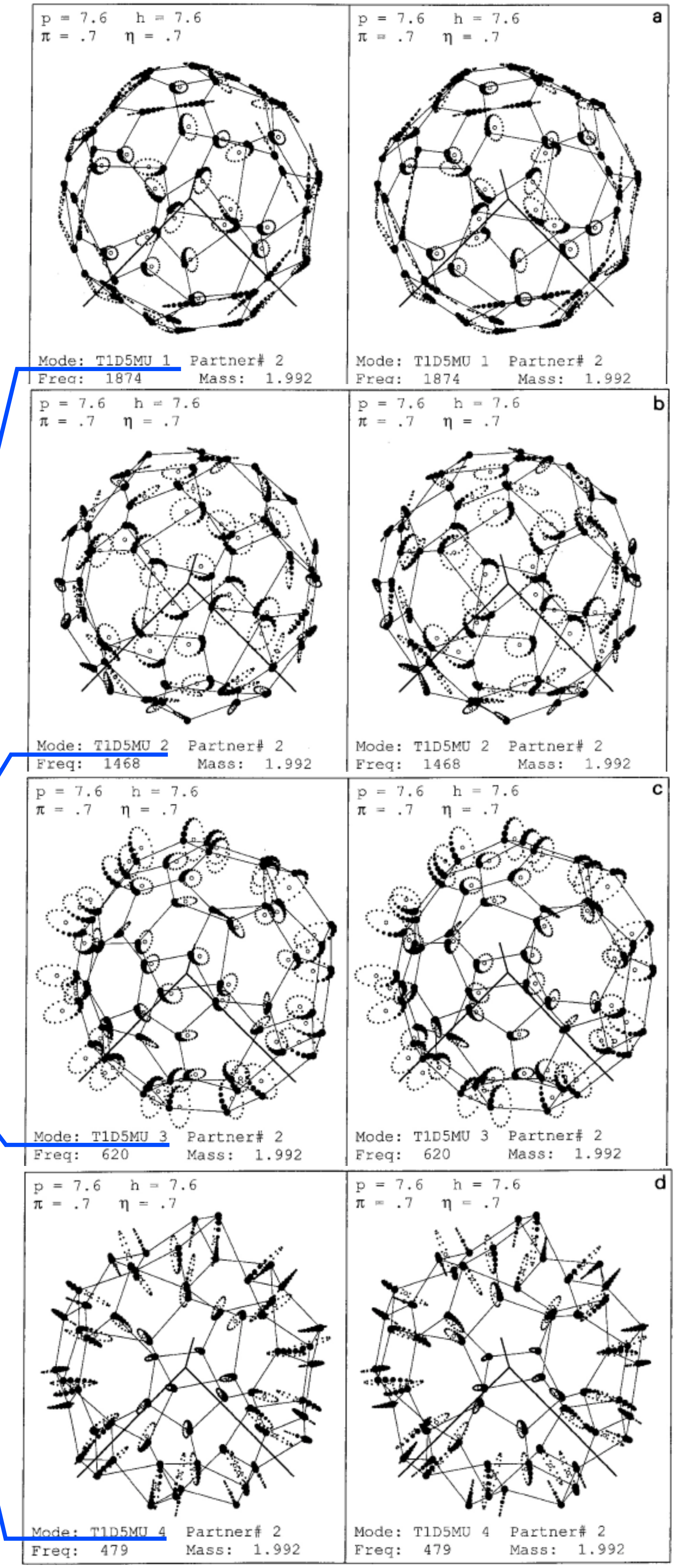
$$\zeta_2^{T_{1u}} = -0.31933$$

$$\zeta_3^{T_{1u}} = -0.49757$$

$$\zeta_4^{T_{1u}} = -0.10698$$

$$\sum_{i=1}^{4} \zeta_i^{T_{1u}} = -1.00001$$





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Scalar Coriolis effects of IR-active C_{60} PQR-bands (Methane to Buckyball)
Comparing vector mode rotation properties in CH_4, CF_4, SF_6, and C_{60}

Table 1
Rovibrational constants and spectral features of CH_4, CF_4, SF_6, and buckyball. Buckyball modes (1)–(4) correspond to modes (a)–(d) in fig. 2

	Molecule							
	CH_4	CF_4	SF_6		buckyball			
	$B=5.3226\ cm^{-1}$ $\nu_3=3020\ cm^{-1}$	$B=0.1854\ cm^{-1}$ $\nu_4=631\ cm^{-1}$	$B=0.09118\ cm^{-1}$		$B=0.00278\ cm^{-1}$			
			$\nu_3=948\ cm^{-1}$	$\nu_4=617\ cm^{-1}$	$\nu_1^{T_{1u}}=1868\ cm^{-1}$	$\nu_2^{T_{1u}}=1462\ cm^{-1}$	$\nu_3^{T_{1u}}=618\ cm^{-1}$	$\nu_4^{T_{1u}}=478\ cm^{-1}$
J_{max} (293 K)								
calculated	6	33	47		266			
observed P branch	7–8	≈30	N/A	≈45	N/A	N/A	N/A	N/A
observed R branch	7–8	≈35	N/A	≈40	N/A	N/A	N/A	N/A
J_{max} (30 K)								
calculated	1	10	15		85			
ζ	0.05	−0.3614	0.6937	−0.2156	−0.0761	−0.3193	−0.4976	−0.1070
$\Delta=2B(1-\zeta)$ (cm^{-1})	10.113	0.505	0.0559	0.222	0.0062	0.0076	0.0086	0.0064
ΔJ_{max} (293 K) (cm^{-1})								
calculated	61	17	2.6	10.4	1.7	2.0	2.3	1.7
observed P branch	≈70	≈16	N/A	≈10	N/A	N/A	N/A	N/A
observed R branch	≈70	≈18	N/A	≈10	N/A	N/A	N/A	N/A
ΔJ_{max} (30 K) (cm^{-1})								
calculated	10	5.05	0.84	3.33	0.527	0.646	0.731	0.544
P, R branch peak to peak (293 K) (cm^{-1})								
calculated	122	34	5.25	21	3.4	4.0	4.6	3.4
observed	140	≈34	N/A	≈20	N/A	N/A	N/A	N/A
peak to peak (30 K) (cm^{-1})								
calculated	20	10.1	1.68	6.66	1.054	1.292	1.462	1.088

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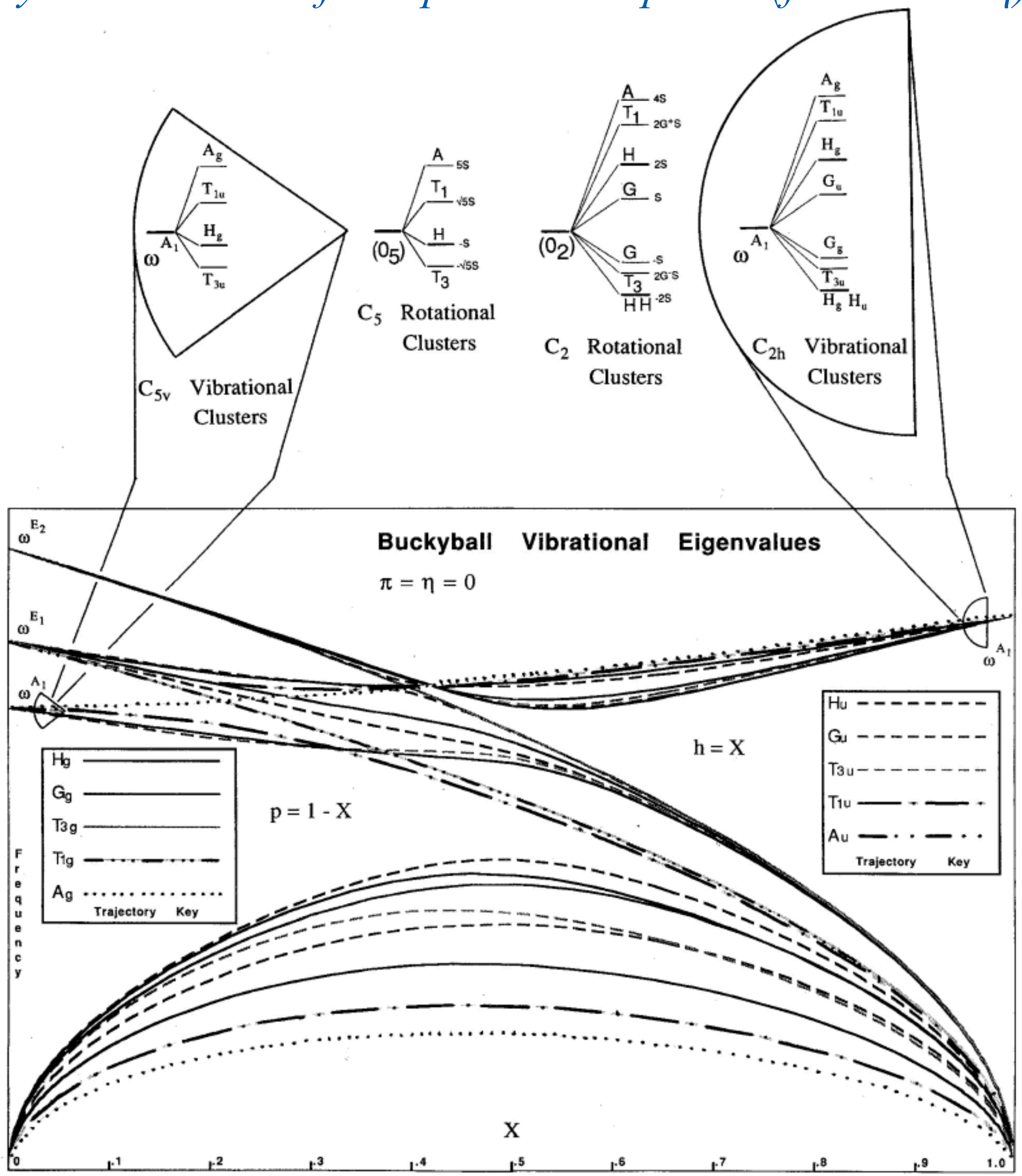
Mode frequency variation with force parameters p=1-h (fixed π=0=η) shows clustering



Weeks,Harter JCP90 pdf p.21

Simpler D_5 pentagonal modes help to check C_{60} system

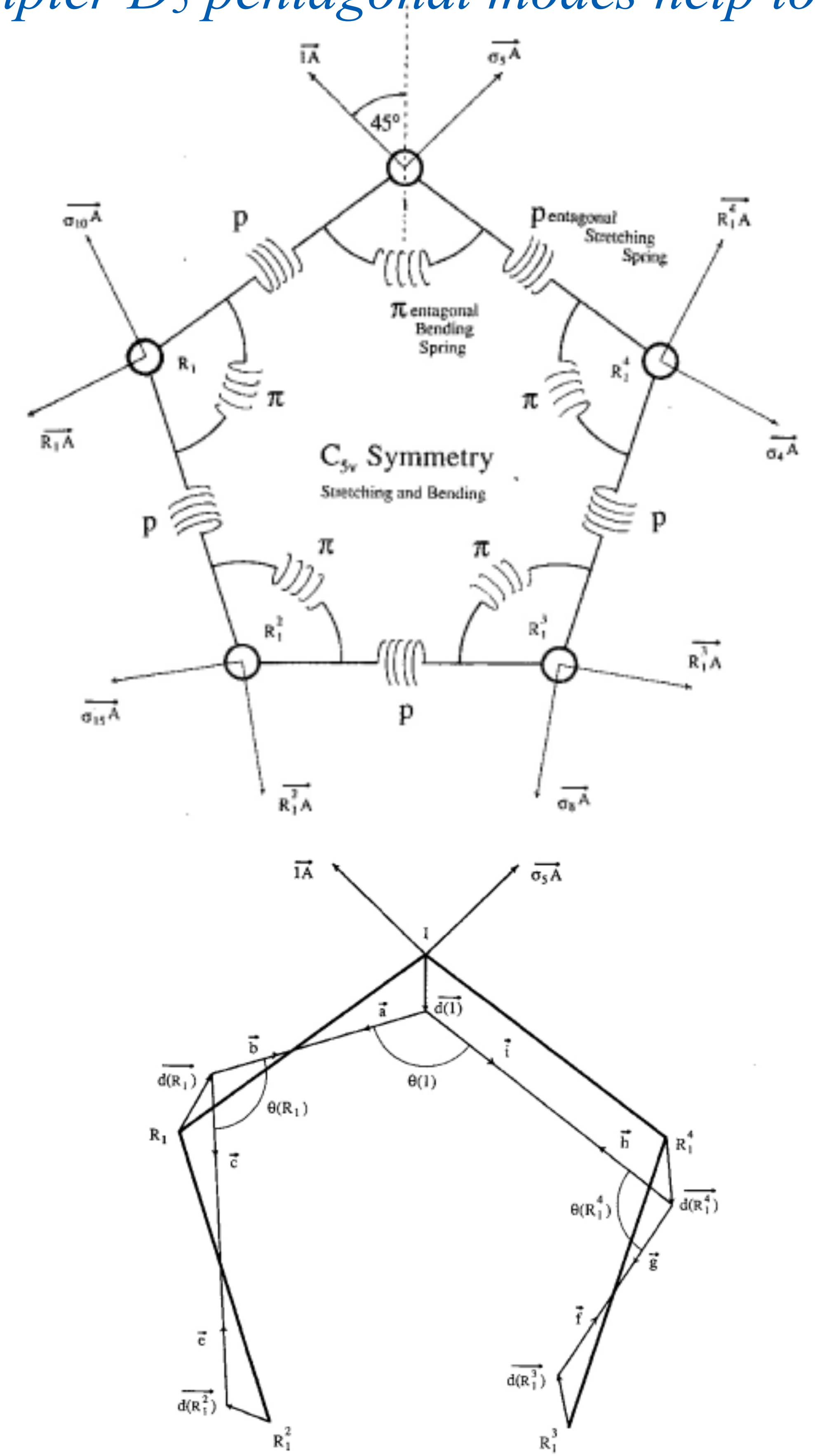


FIG. 19. (a) A C_{5v} symmetric spring-mass model with stretching and bending springs. (b) The unit cell of C_{5v} symmetric spring-mass model. Displacement vectors $\vec{d(g)}$, edge vectors, $\vec{a}, \vec{b},\ldots,\vec{i}$, and angles $\theta(g)$ used in the calculation of the potential are labeled.

TABLE IV. (a) Displacement vectors $d(g)$ used in the calculation of the edge vectors. (b) Edge vectors used to calculate angles.

(a)

$$\vec{a} = \hat{a} - d(1) + d(R_1) \qquad \vec{f} = \hat{f} - d(R_1^3) + d(R_1^4)$$
$$\vec{b} = \hat{b} - d(R_1) + d(1) \qquad \vec{g} = \hat{g} - d(R_1^4) + d(R_1^3)$$
$$\vec{c} = \hat{c} - d(R_1) + d(R_1^2) \qquad \vec{h} = \hat{h} - d(R_1^4) + d(1)$$
$$\vec{e} = \hat{e} - d(R_1^2) + d(R_1) \qquad \vec{i} = \hat{i} - d(1) + d(R_1^4)$$

(b)

$$\theta(1) = \arccos\left\{\frac{\vec{a}\cdot\vec{i}}{|\vec{a}||\vec{i}|}\right\}$$

$$\theta(R_1) = \arccos\left\{\frac{\vec{b}\cdot\vec{c}}{|\vec{b}||\vec{c}|}\right\}$$

$$\theta(R_1^4) = \arccos\left\{\frac{\vec{g}\cdot\vec{h}}{|\vec{g}||\vec{h}|}\right\}$$

TABLE V. C_{5v} force matrix elements as a function of stretching and bending. Results of numerical and analytical calculations are given where $\theta = 81°$ and $\phi = 9^0$.

Force matrix elements	Numerical results stretching + bending	Analytic results stretching + bending
$\langle 1A \vert F \vert 1A\rangle$	$= 1.000\,0000p + 2.309\,0170\pi$	$= p + (2 - G^-/2)\pi$
$\langle 1A \vert F \vert R_1 A\rangle$	$= -0.154\,5085p - 1.309\,0170\pi$	$= pG^-/4 + (G^-/2 - 1)\pi$
$\langle 1A \vert F \vert R_1^2 A\rangle$	$= 0.000\,0000p + 0.154\,5085\pi$	$= 0p - \pi G^-/4$
$\langle 1A \vert F \vert R_1^3 A\rangle$	$= 0.000\,0000p + 0.154\,5085\pi$	$= 0p - \pi G^-/4$
$\langle 1A \vert F \vert R_1^4 A\rangle$	$= -0.154\,5085p - 1.309\,0170\pi$	$= pG^-/4 + (G^-/2 - 1)\pi$
$\langle 1A \vert F \vert \sigma_5 A\rangle$	$= -0.309\,0170p + 1.618\,03440\pi$	$= pG^-/2 + \pi G^+$
$\langle 1A \vert F \vert \sigma_{10} A\rangle$	$= 0.024\,4717p - 2.260\,0735\pi$	$= p\cos^2\theta + (\sqrt{2}\cos\phi/G^-)\pi$
$\langle 1A \vert F \vert \sigma_{15} A\rangle$	$= 0.000\,0000p + 0.975\,5283\pi$	$= 0p + \pi\cos^2\phi$
$\langle 1A \vert F \vert \sigma_8 A\rangle$	$= 0.000\,0000p + 0.024\,4717\pi$	$= 0p + \pi\cos^2\theta$
$\langle 1A \vert F \vert \sigma_4 A\rangle$	$= 0.975\,5283p - 0.357\,9604\pi$	$= p\cos^2\phi + (\sqrt{2}\cos\theta/G^-)\pi$

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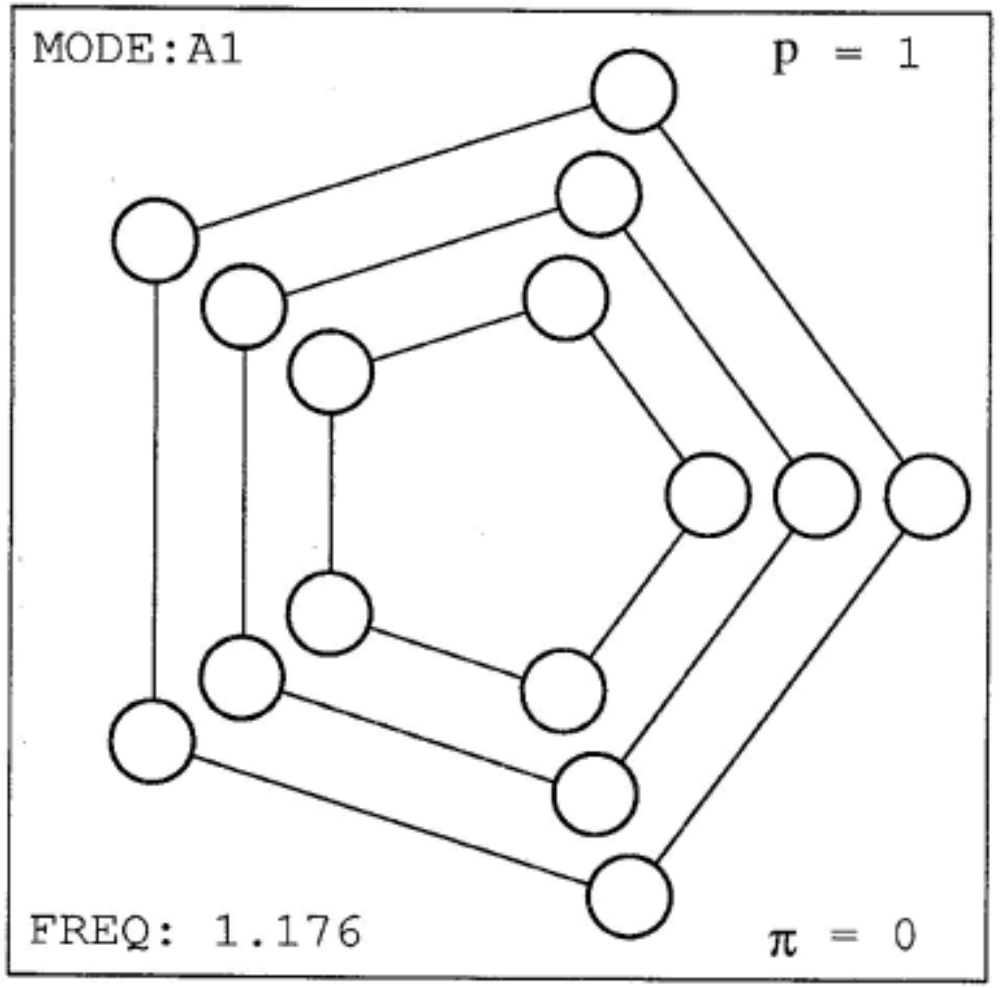

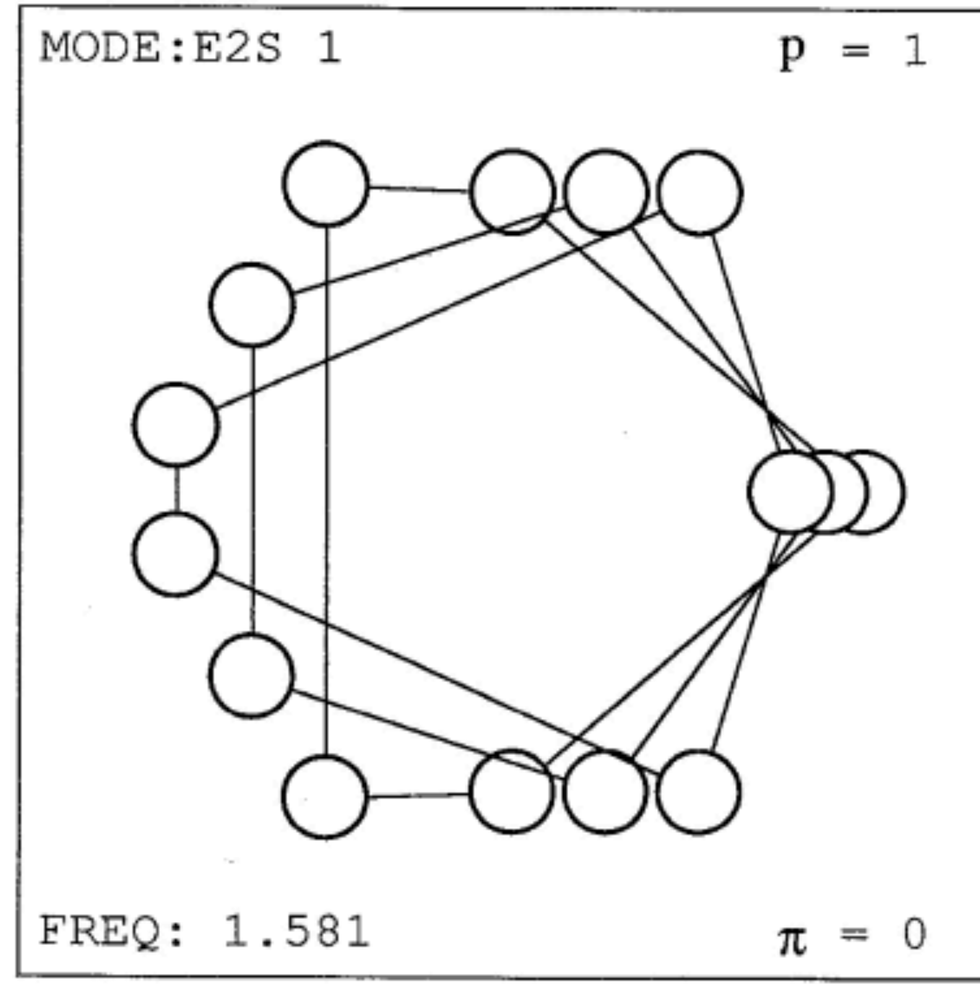

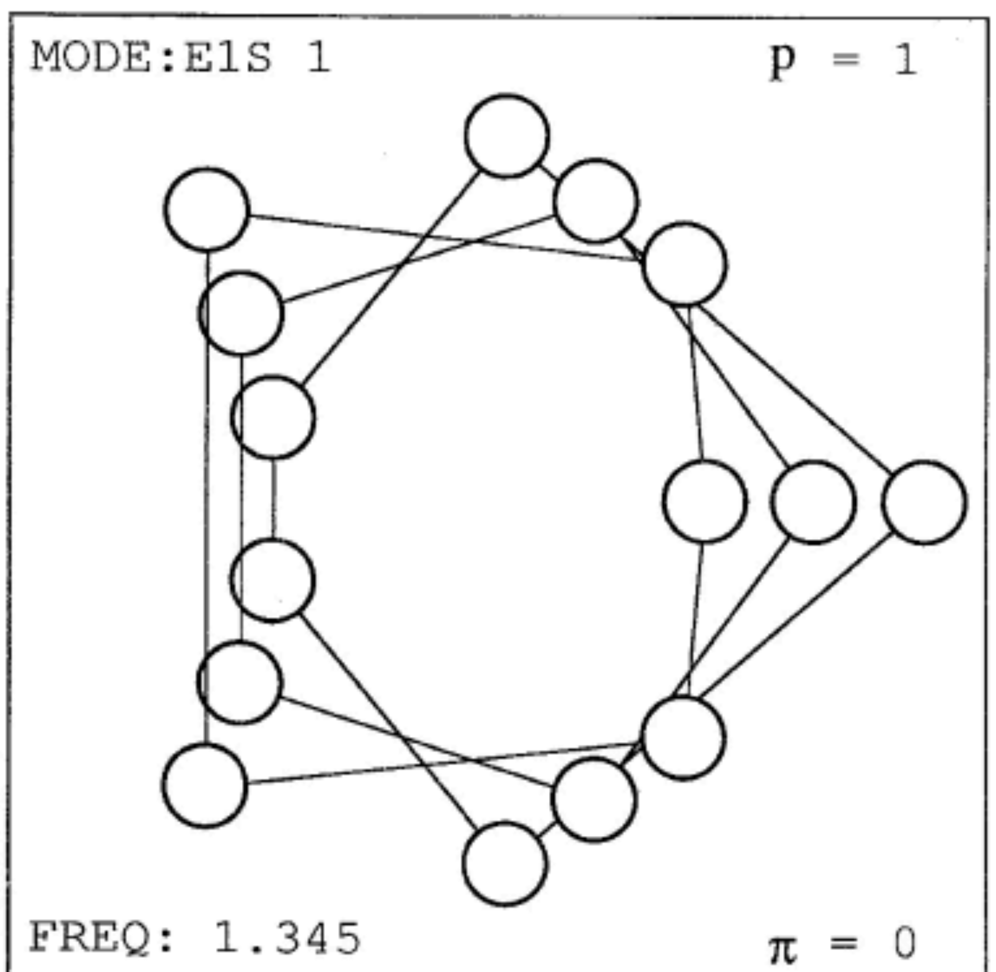

FIG. 20. Normal modes of the C_{5v} symmetric spring-mass model defined by the C_{5v}, C_v subgroup chain. Each mode varies as $\cos(\omega t)$ and is plotted at time $t = 0$, $t = \pi/2\omega$, and $t = \pi/\omega$. (a) The A_1 "breathing" mode, (b) One of two nonzero frequency vector E_1 modes, and (c) One of two nonzero frequency E_2 modes.

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AMOP reference links on pages 2-4

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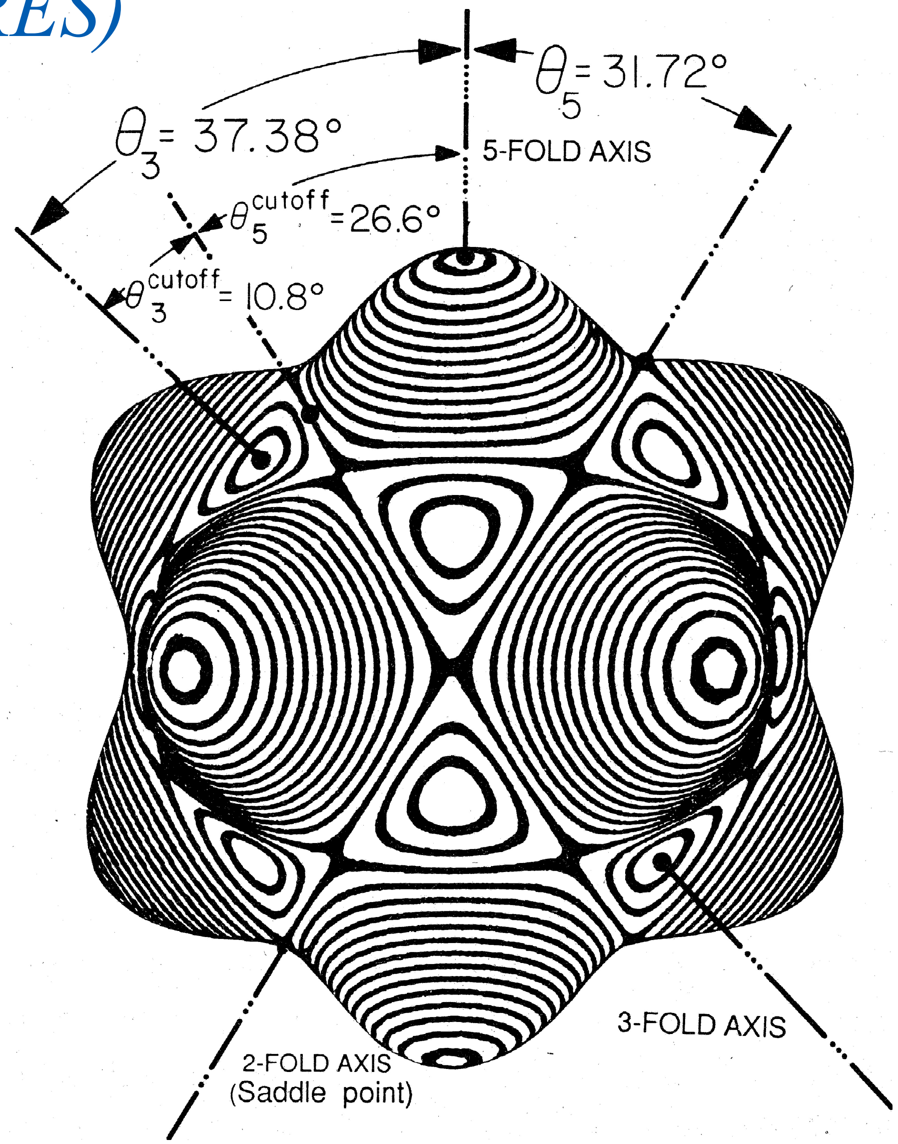
Tensor centrifugal tensor effects for high-J rotation of C_{60}
Rotational-Energy-Surfaces (RES)

Lowest rank tensor $\mathbf{T}^{[k]}=\mathbf{T}^{[6]}$ that has *icosahedral* symmetry:

$$\mathbf{T}^{[6]}=\frac{\sqrt{11}}{5}\mathbf{T}^{6}_{0}+\frac{\sqrt{7}}{5}\left(\mathbf{T}^{6}_{+5}-\mathbf{T}^{6}_{-5}\right)$$



I-Tensors Harter,Weeks JCP90 pdf p.2

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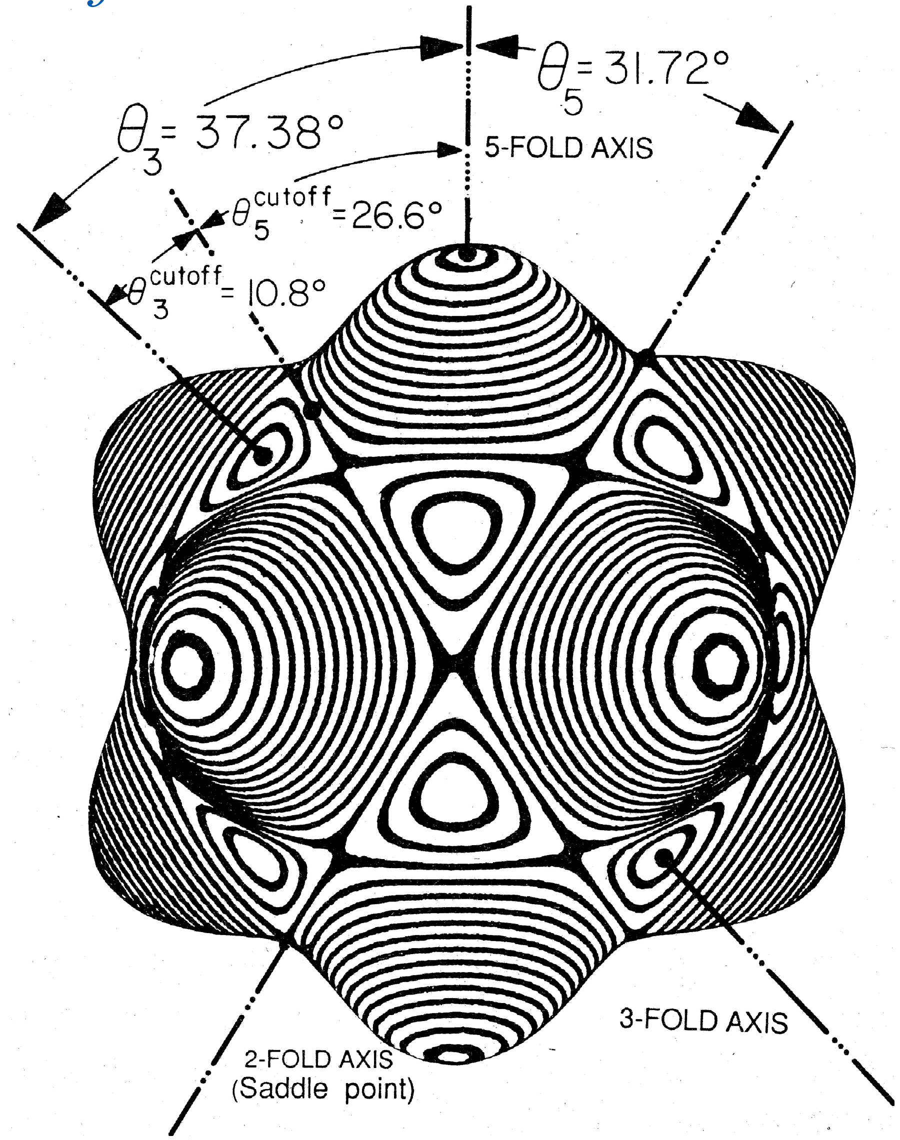
$$\mathbf{T}^{[6]} = \frac{\sqrt{11}}{5}\mathbf{T}_0^6 + \frac{\sqrt{7}}{5}\left(\mathbf{T}_{+5}^6 - \mathbf{T}_{-5}^6\right)$$



Polar coordinate function for $\mathbf{T}^{[6]}$ RES

$$T^{[6]}(\theta,\phi) =$$

$$J^6\frac{\sqrt{11}}{80}\left[\left(231\cos^6\theta - 315\cos^4\theta - 105\cos^2\theta - 5\right) - 42\cos\theta\sin^5\phi\cos\phi\left(16\cos^4\phi - 20\cos^2\phi + 5\right)\right]$$

Tensor centrifugal tensor effects for high-J rotation of C_{60}
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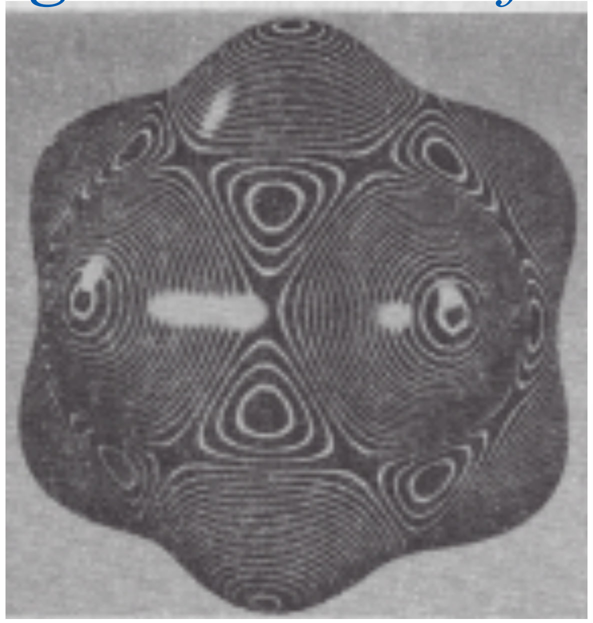
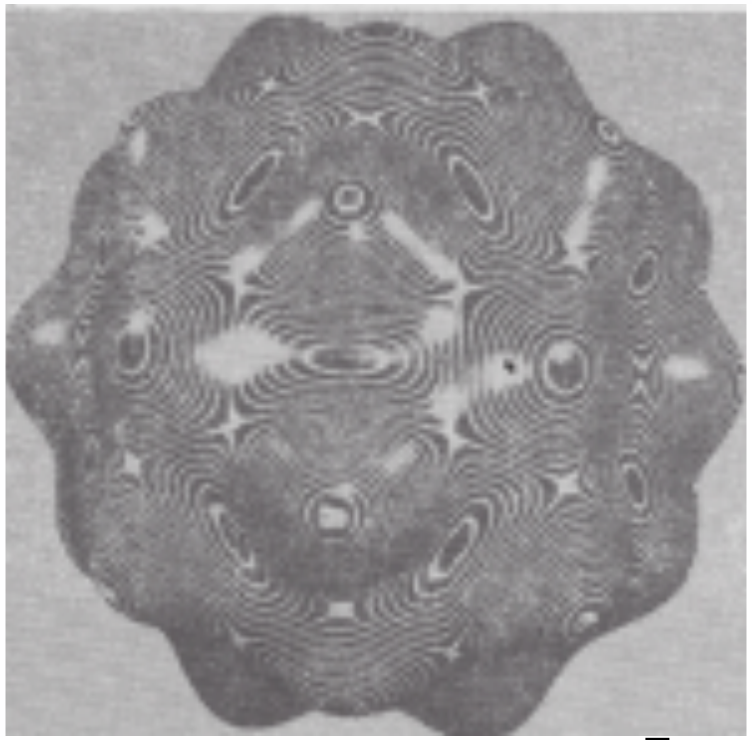


Lowest rank tensor $\mathbf{T}^{[k]}=\mathbf{T}^{[6]}$ that has *icosahedral* symmetry:

$$\mathbf{T}^{[6]} = \frac{\sqrt{11}}{5}\mathbf{T}^{6}_{0} + \frac{\sqrt{7}}{5}\left(\mathbf{T}^{6}_{+5} - \mathbf{T}^{6}_{-5}\right)$$

Next lowest rank tensor $\mathbf{T}^{[k]}=\mathbf{T}^{[10]}$ is:



$$\mathbf{T}^{[10]} = \frac{\sqrt{3\cdot 13\cdot 19}}{75}\mathbf{T}^{10}_{0} - \frac{\sqrt{11\cdot 19}}{25}\left(\mathbf{T}^{10}_{+5} - \mathbf{T}^{10}_{-5}\right) + \frac{\sqrt{3\cdot 11\cdot 17}}{75}\left(\mathbf{T}^{10}_{+10} - \mathbf{T}^{10}_{-10}\right)$$

Polar coordinate function for $\mathbf{T}^{[6]}$ RES

$$T^{[6]}(\theta,\phi) =$$

$$J^{6}\frac{\sqrt{11}}{80}\left[\left(231\cos^{6}\theta - 315\cos^{4}\theta - 105\cos^{2}\theta - 5\right) - 42\cos\theta\sin^{5}\phi\cos\phi\left(16\cos^{4}\phi - 20\cos^{2}\phi + 5\right)\right]$$

I-Tensors Harter,Weeks JCP90 pdf p.2

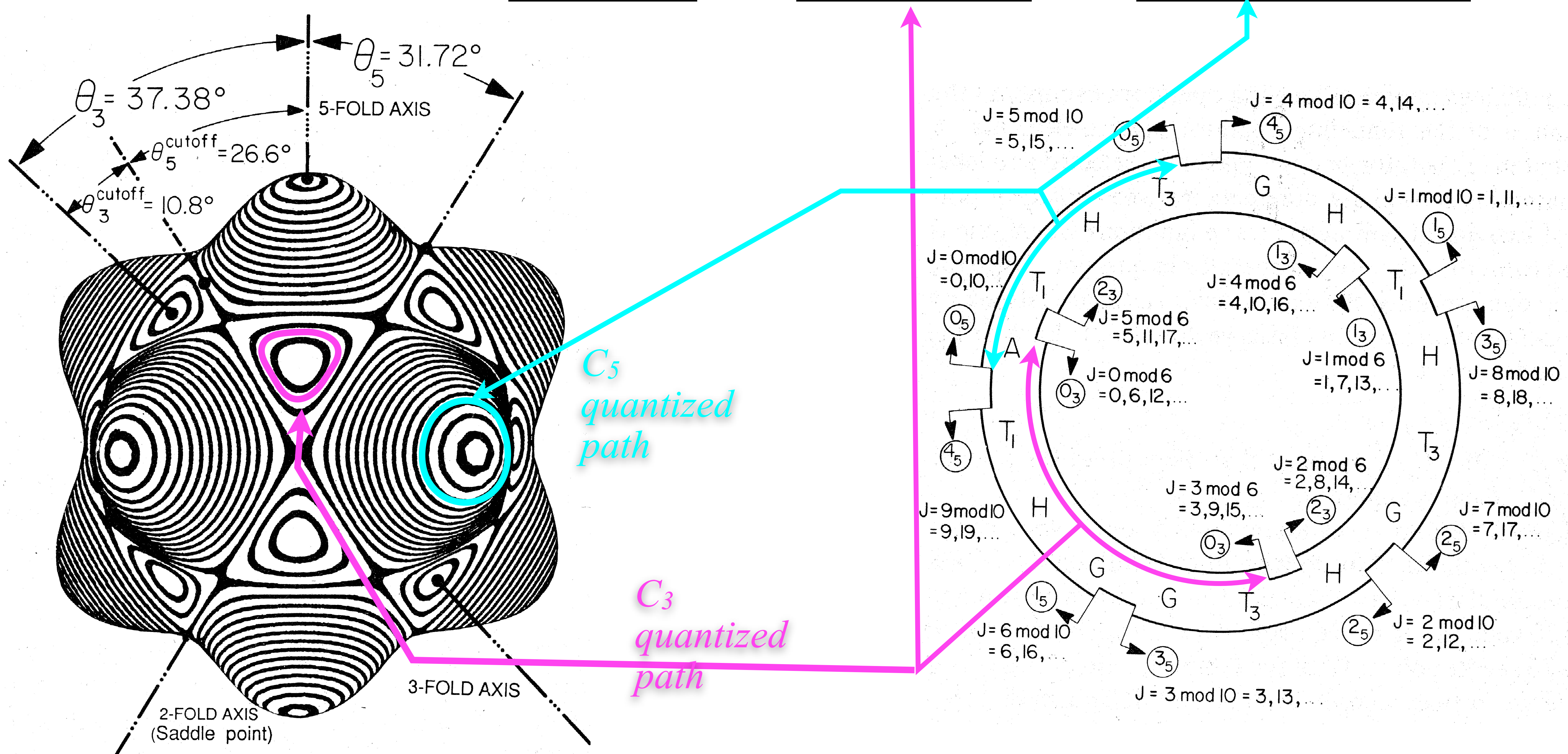
Eigenstates of **T**[6] *belong to* (m3 of C3)↑*I and (mainly) to* (m5 of C5)↑*I*

Rotational correlations for J-orbits about RES hills or valleys:

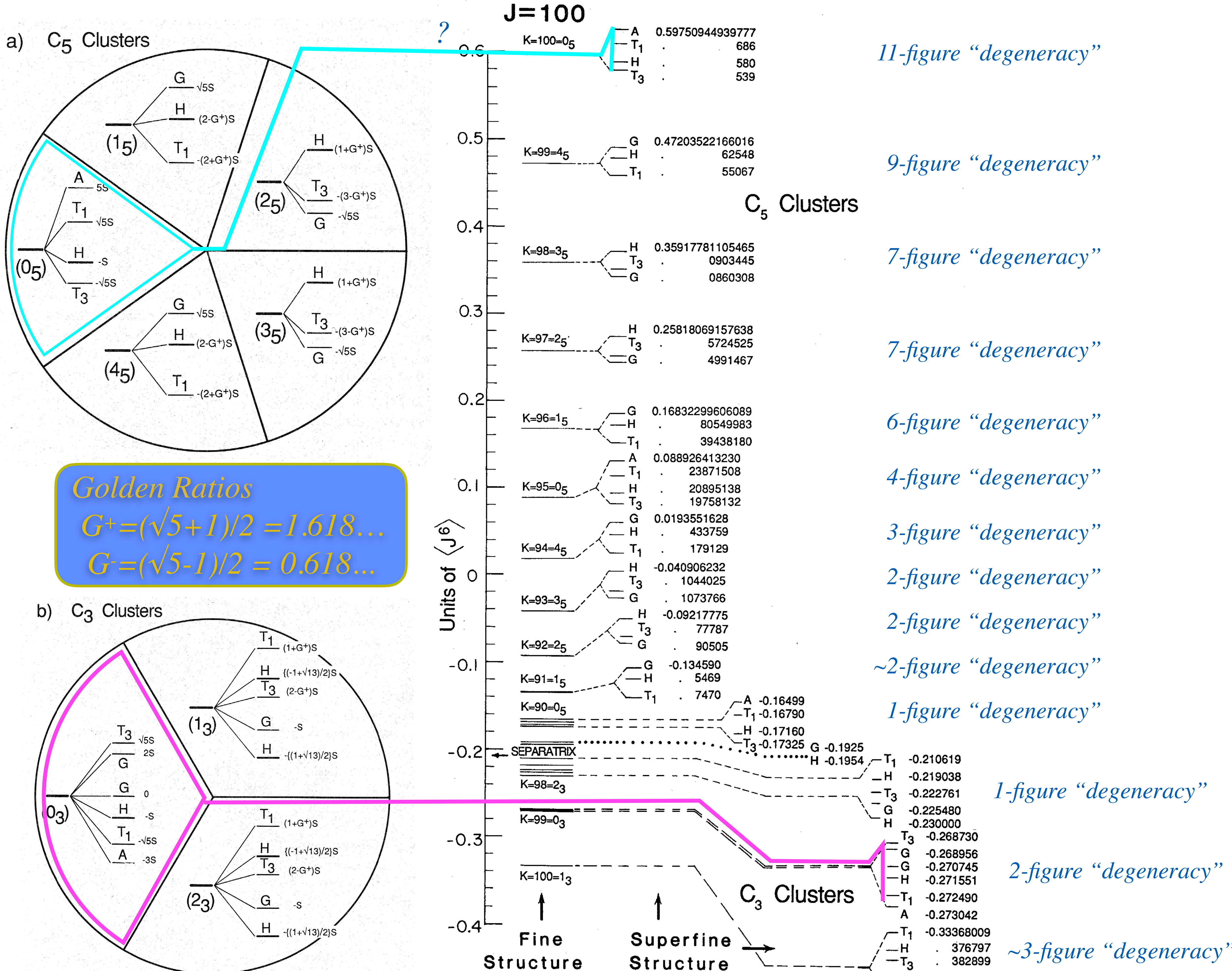
$I\supset C_2$	0_2	1_2
A	1	·
T_1	1	2
T_3	1	2
G	2	2
H	3	2

$I\supset C_3$	0_3	1_3	2_3
A	1	·	·
T_1	1	1	1
T_3	1	1	1
G	2	1	1
H	1	2	2

$I\supset C_5$	0_5	1_5	2_5	3_5	4_5
A	1	·	·	·	·
T_1	1	1	·	·	1
T_3	1	·	1	1	·
G	·	1	1	1	1
H	1	1	1	1	1



I-Tensors Harter, Weeks JCP90 pdf p.9



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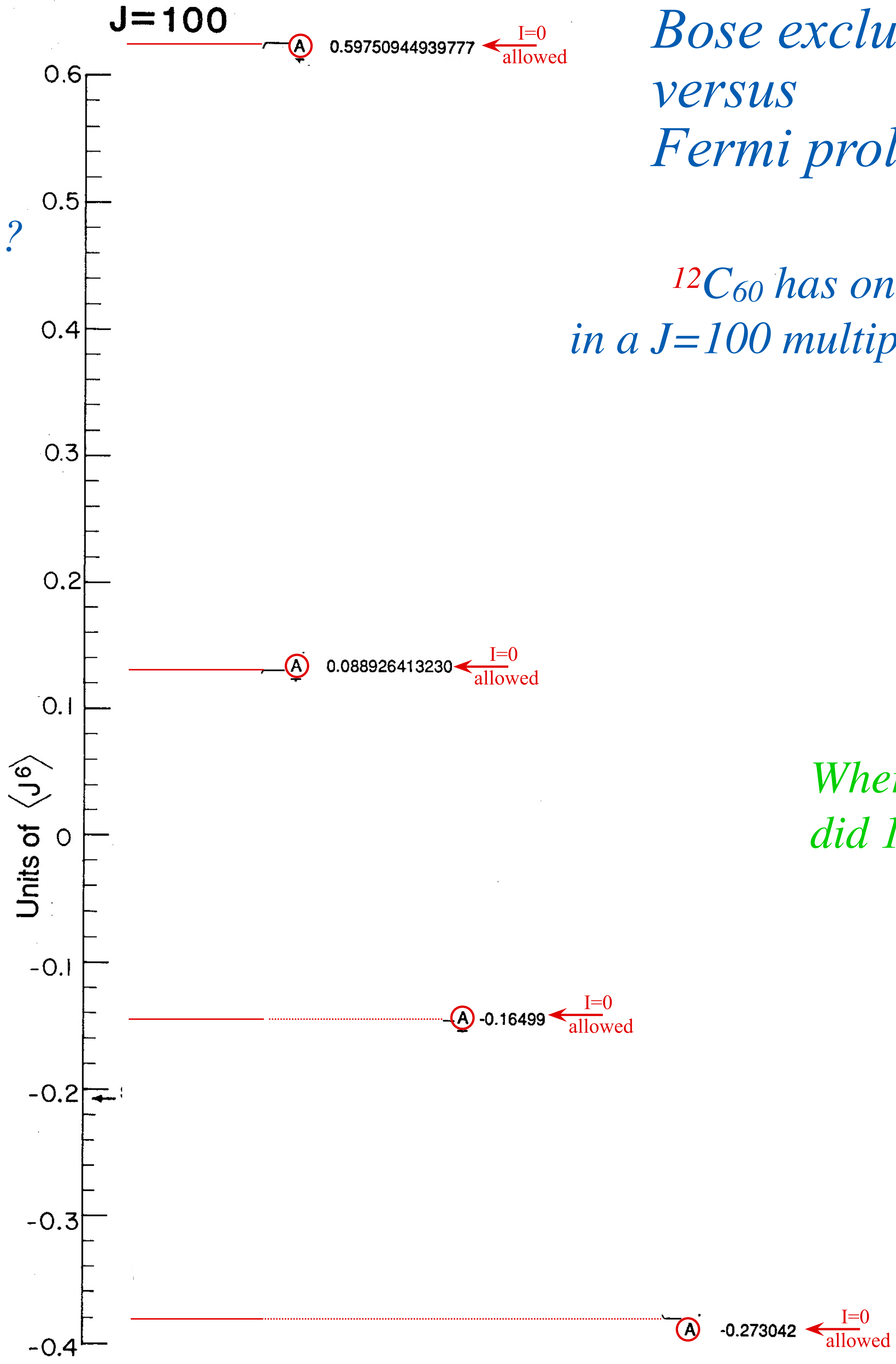
Example of ??μm spectra of $^{12}C_{60}$?



$^{12}C_{60}$ has on 4 allowed states in a J=100 multiplet of 201=2J+1

Where the !#@$% did 197 states go??!!

Bose exclusion in $^{12}C_{60}$
versus
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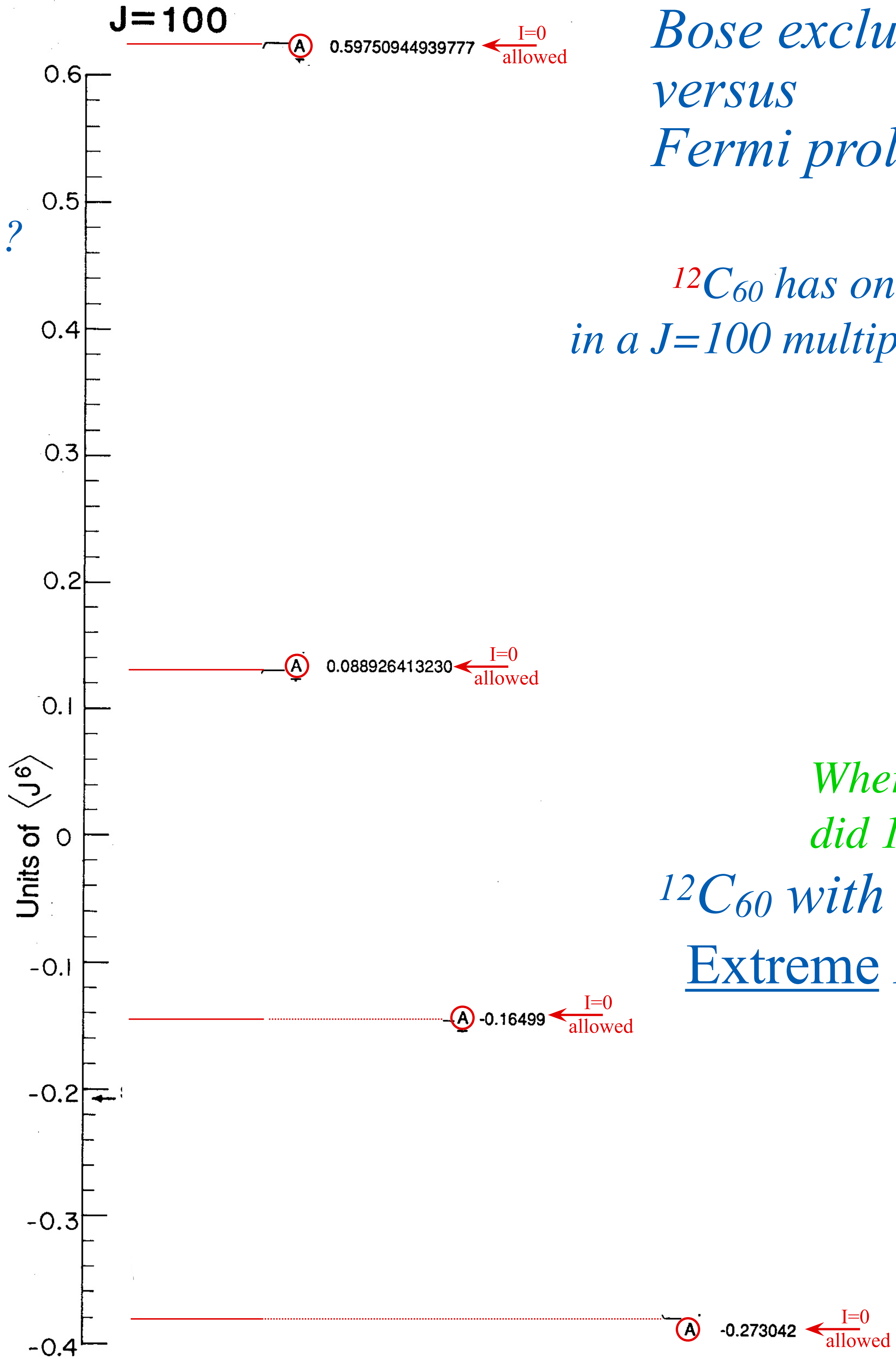
Example of ??μm spectra of $^{12}C_{60}$?



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Where the !#@$%
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$^{12}C_{60}$ with spin-0 nuclei has
Extreme *Bose Exclusion!*

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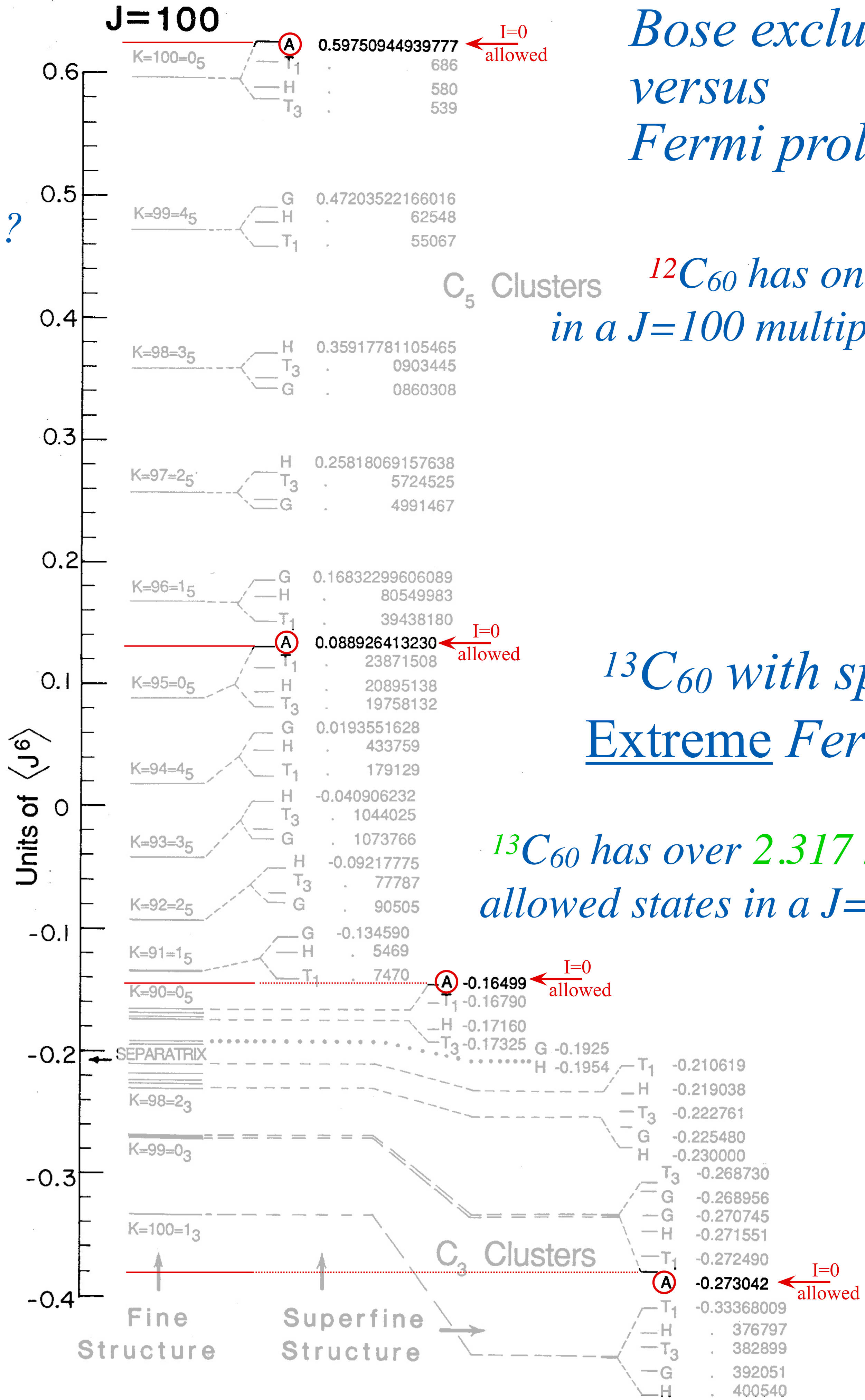

$^{12}C_{60}$ has on 4 allowed states in a J=100 multiplet of 201=2J+1

$^{13}C_{60}$ with spin-½ nuclei has <u>Extreme</u> *Fermi Proliferation!*

$^{13}C_{60}$ has over 2.317 hundred octillion allowed states in a J=100 multiplet of 201

$2^{60}=1.5292 \cdot 10^{18}$

Bose exclusion in $^{12}C_{60}$
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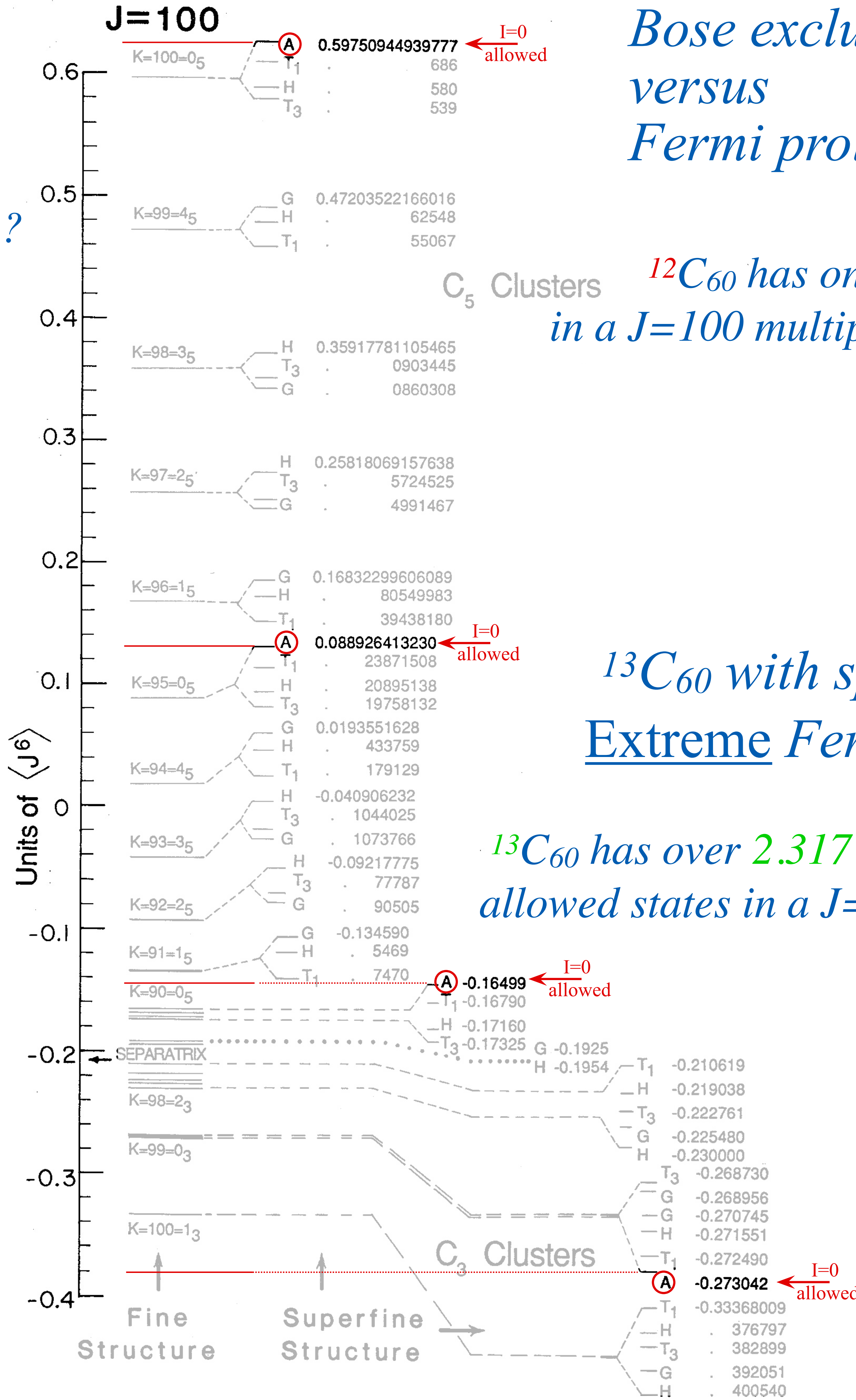
Example of ??µm spectra of $^{12}C_{60}$?



$^{12}C_{60}$ has on 4 allowed states
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The good news…
$^{13}C_{60}$ has only
N=10 times as many
nuclei as SF_6

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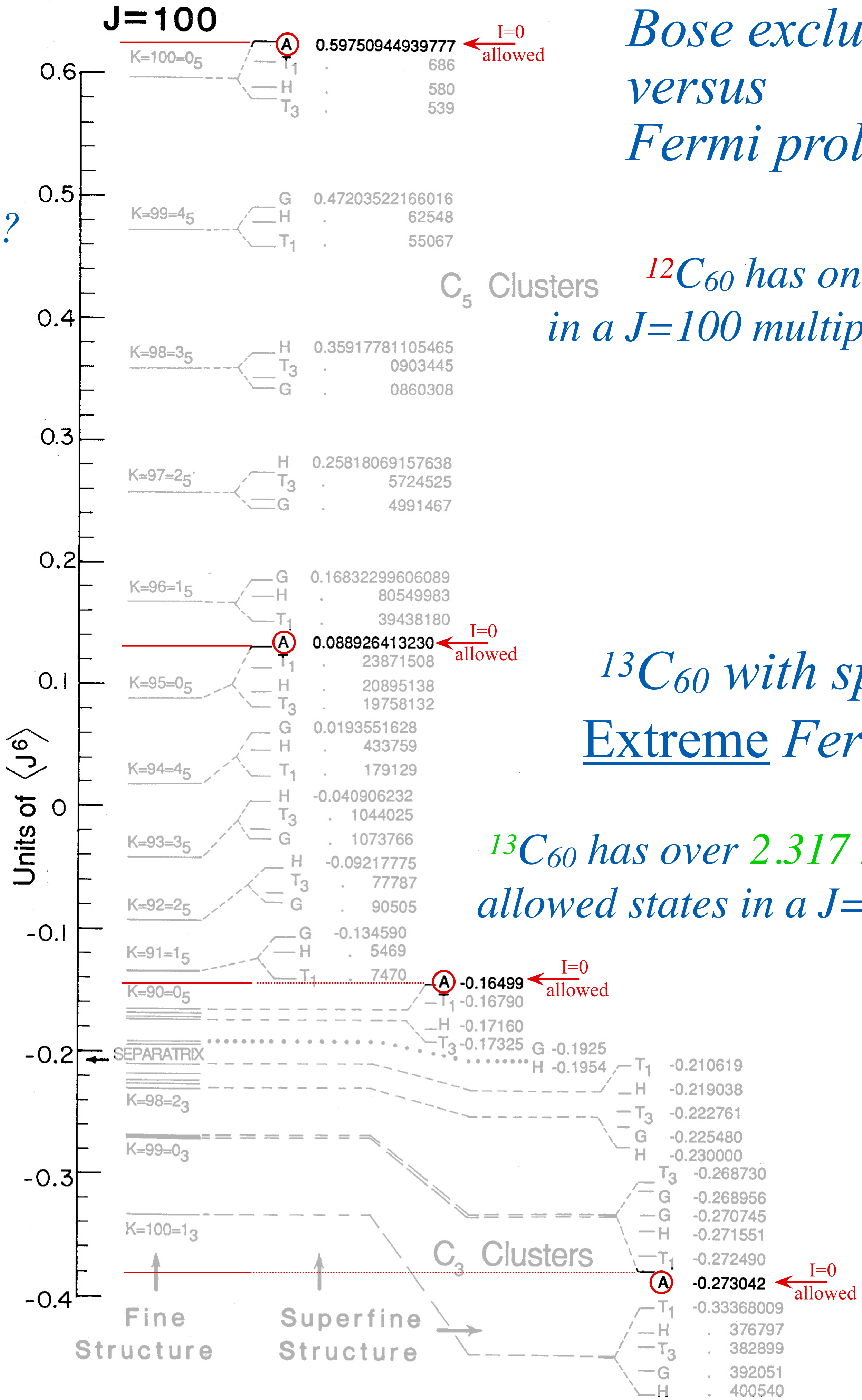

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The bad news…
that number N=10 is in the EXPONENT!!

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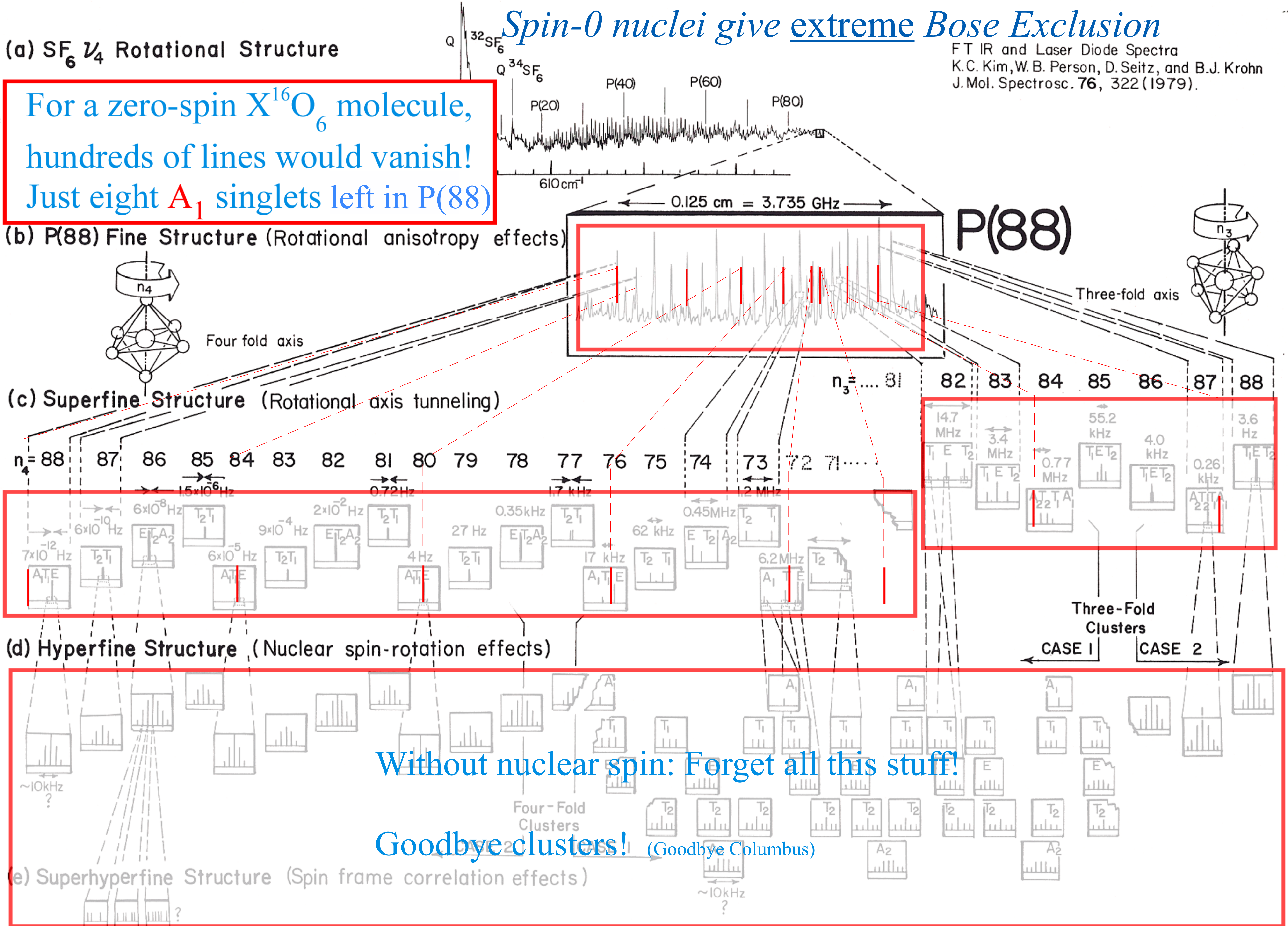
Spin-0 nuclei give extreme Bose Exclusion

For a zero-spin $X^{16}O_6$ molecule, hundreds of lines would vanish! Just eight A_1 singlets left in P(88)



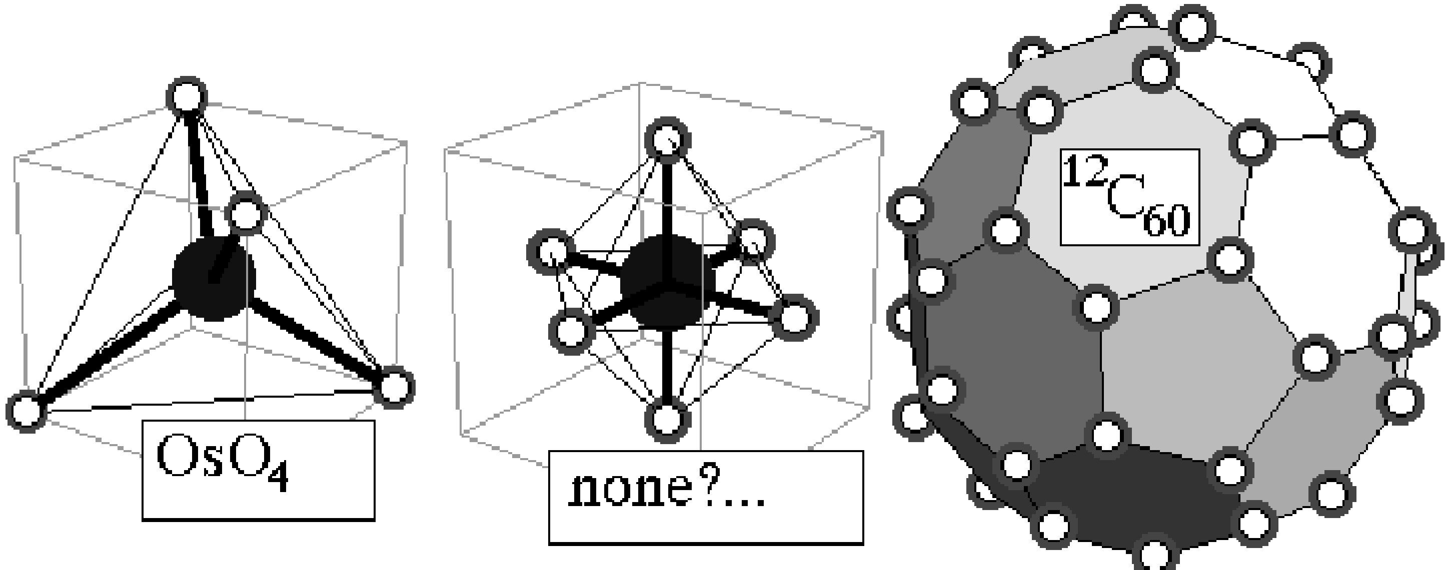
Without nuclear spin: Forget all this stuff!

Goodbye clusters! (Goodbye Columbus)

Spin-0 nuclei give extreme Bose Exclusion

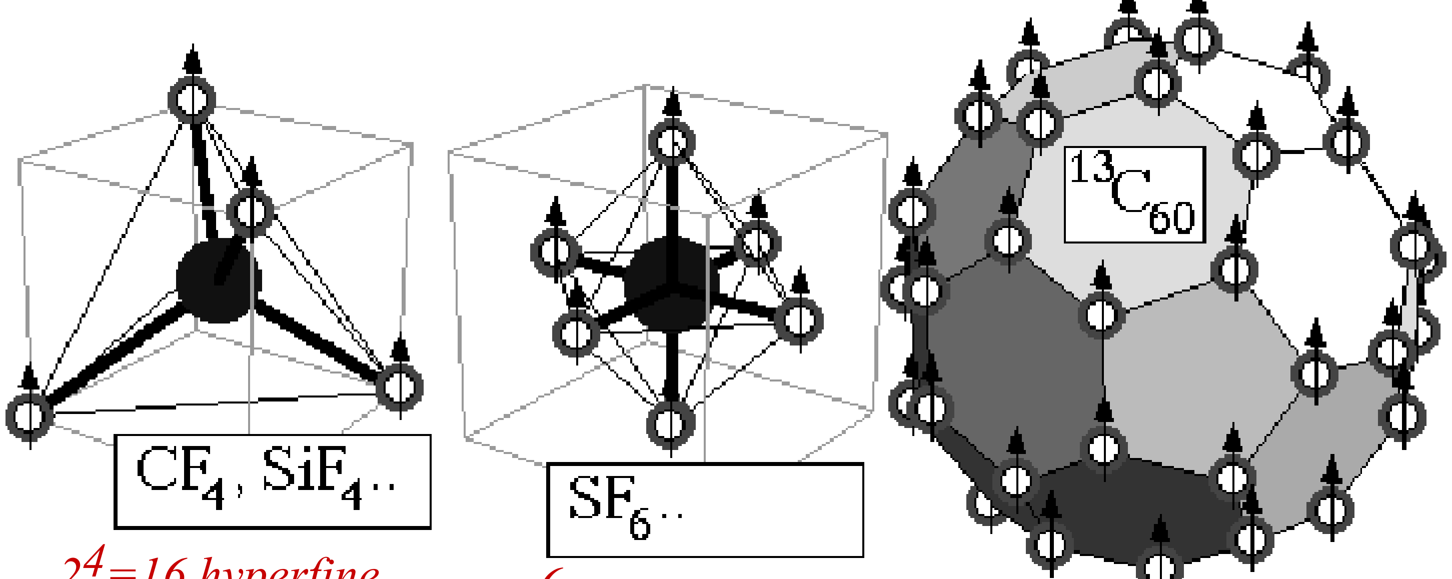
Some examples of Bose Exclusion

Spherical Top Molecules with Spin-0 Nuclei



Only 1 hyperfine state: I=0

Spherical Top Molecules with Spin-1/2 Nuclei



2^4=16 hyperfine states: I=0-2

2^6=64 hyperfine states: I=0-3

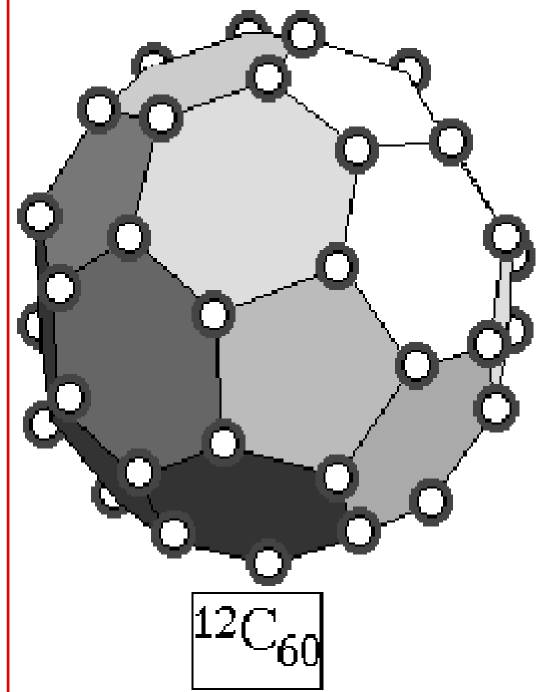
2^{60}=1.15x10^{18} hyperfine states: I=0-30

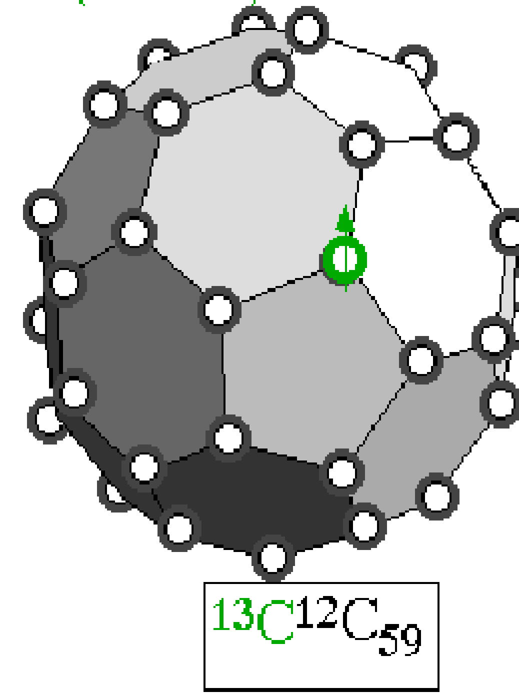
Some examples of Fermi (non) Exclusion

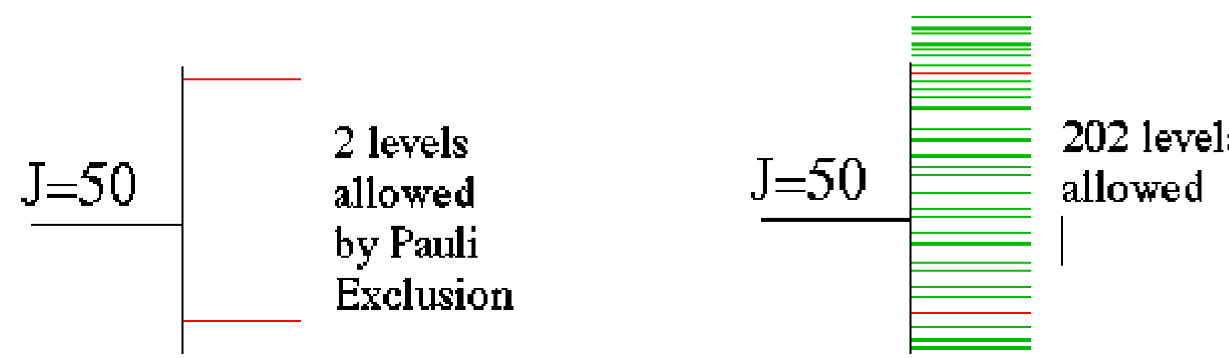
Example of extreme symmetry exclusion

... (and partial recovery)

Y_h Symmetry reduced to C_v by a single neutron (in ^{13}C)

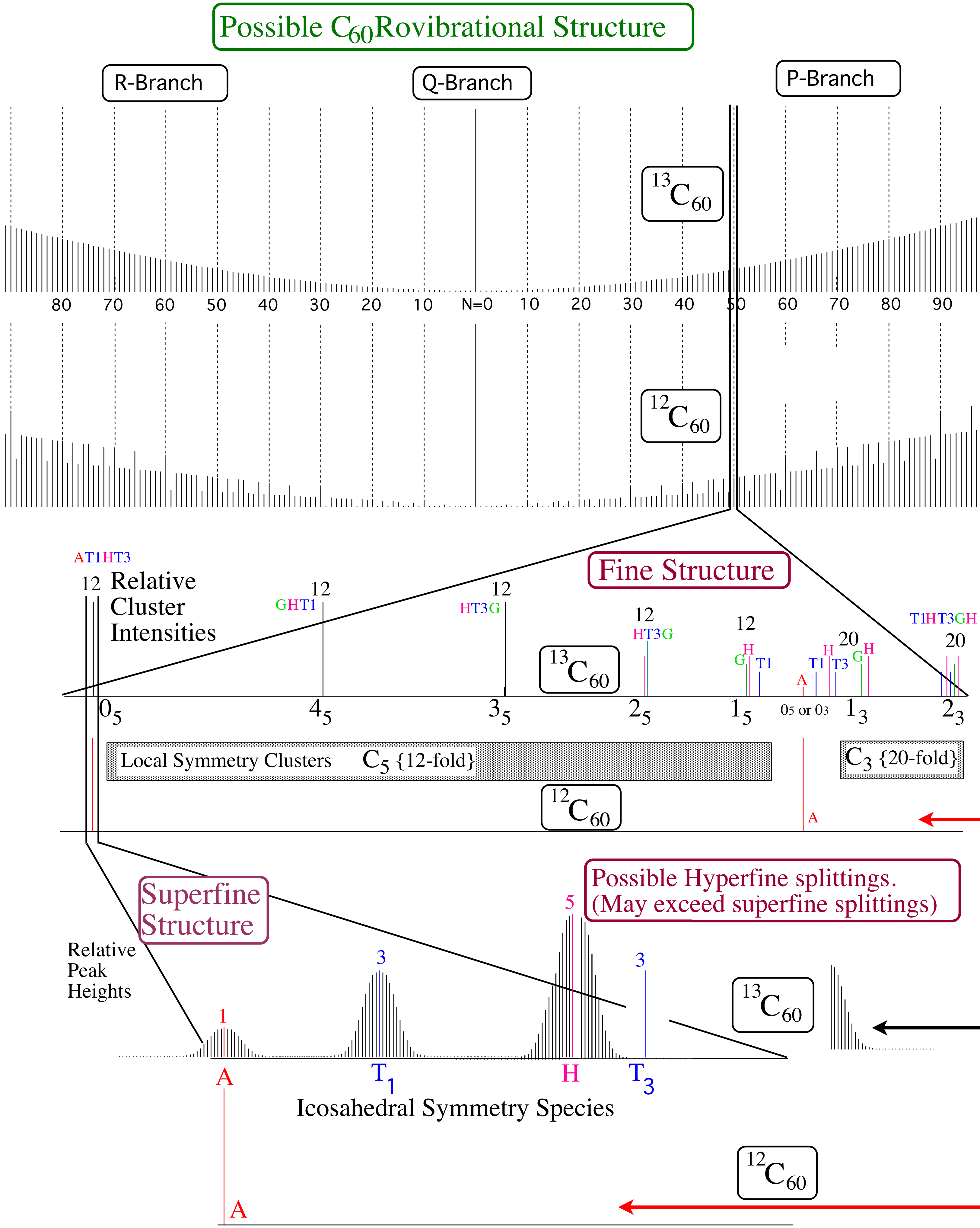






Question: Where did those 200 levels go?

Better Question: Where did those 1.15 octillion levels go?



W.G.Harter, D.E.Weeks,
Chem. Phys. Letters 194,3(1992)pdf p.4

J=50
Fine structure
comparing
$^{13}C_{60}$ (2^{60} Hyperfine levels)

with
$^{12}C_{60}$ (1^{60} Hyperfine level)

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I	Par	A (A_g, A_u)	T_1 (T_{1g}, T_{1u})	T_3 (T_{3g}, T_{3u})	G (G_g, G_u)	H (H_g, H_u)
30	g	1	0	0	0	0
	u	0	0	0	0	0
29	g	0	1	1	2	3
	u	0	2	2	2	2
28	g	22	36	36	58	80
	u	14	42	42	56	70
27	g	280	804	804	1084	1354
	u	260	826	826	1086	1336
26	g	3887	11238	11238	15125	19022
	u	3772	11324	11324	15096	18878
25	g	41528	124257	124257	165779	207307
	u	41266	124548	124548	165808	207074
24	g	372752	1114158	1114158	1486916	1859568
	u	371694	1114942	1114942	1486642	1858246
23	g	2801748	8402852	8402852	11204600	14006448
	u	2799558	8405316	8405316	11204874	14004522
22	g	18110340	54304371	54304371	72414711	90525051
	u	18103410	54309474	54309474	72412884	90516294
21	g	101874363	305608974	305608974	407483337	509357130
	u	101861196	305623968	305623968	407485164	509345790
20	g	505125708	1515241704	1515241704	2020367376	2525493654
	u	505090980	1515266928	1515266928	2020357878	2525449428
19	g	2227563126	6682635360	6682635360	8910198522	11137761648
	u	2227502850	6682705140	6682705140	8910208020	11137710870
18	g	8805633300	26416344630	26416344630	35221977930	44027608785
	u	8805495420	26416442910	26416442910	35221938330	44027431350
17	g	31395905685	94187559795	94187559795	125583465480	156979373610
	u	31395687300	94187817780	94187817780	125583505080	156979194780
16	g	101492436960	304475471640	304475471640	405967908600	507460345560
	u	101491992360	304475780520	304475780520	405967772880	507459765240
15	g	298734989924	896204629630	896204629630	1194939619444	1493674601616
	u	298734348764	896205406510	896205406510	1194939755164	1493674096176
14	g	803453709856	2410356037985	2410356037985	3213809747951	4017263465559
	u	803452525816	2410356831830	2410356831830	3213809357756	4017261891324
13	g	1980110898945	5940332333550	5940332333550	7920443232495	9900554131440
	u	1980109351620	5940334271070	5940334271070	7920443622690	9900552974310
12	g	4481735502630	13445194549380	13445194549380	17926930052010	22408665535200
	u	4481732871390	13445196226770	13445196226770	17926929098160	22408661950230
11	g	9331438352730	27994315570980	27994315570980	37325753923710	46657192295880
	u	9331435261110	27994319616450	27994319616450	37325754877560	46657190157990
10	g	17892025439775	53676052490265	53676052490265	71568077929785	89460103369560
	u	17892020535870	53676055391160	53676055391160	71568075926790	89460096462660
9	g	31605175642230	94815530686980	94815530686980	126420706329465	158025881932935
	u	31605170531130	94815537801090	94815537801090	126420708332460	158025878824830
8	g	51415130846760	154245351765540	154245351765540	205660482612300	257075613497820
	u	51415123186380	154245355784100	154245355784100	205660478970480	257075602195620
7	g	76925432220000	230776308338940	230776308338940	307701740558940	384627172778940
	u	76925425313100	230776318887660	230776318887660	307701744200760	384627169513860
6	g	105558807981090	316676363633175	316676363633175	422235171614265	527793979532265
	u	105558798039270	316676367808710	316676367808710	422235165847980	527793963824370
5	g	132192080280555	396576266554074	396576266554074	528768346834233	660960427177878
	u	132192072923730	396576279677184	396576279677184	528768352600518	660960425587128
4	g	149756091280506	449268197030424	449268197030424	599024288311326	748780379591832
	u	149756080818726	449268199508214	449268199508214	599024280327336	748780361146062
3	g	150988619146706	452965902231668	452965902231668	603954521378374	754943140441100
	u	150988613640506	452965915721858	452965915721858	603954529362364	754943142918890
2	g	130959549507485	392878564027270	392878564027270	523838113534755	654797663126220
	u	130959541149860	392878562690050	392878562690050	523838103839910	654797645073750
1	g	89413728633564	268241251090167	268241251090167	357654979723731	447068708357295
	u	89413727296344	268241262122232	268241262122232	357654989418576	447068716714920
0	g	31791575566072	95374646372040	95374646372040	127166221937640	158957797411208
	u	31791571643468	95374639953380	95374639953380	127166211596396	158957783147612

Total nuclear spin-weight of each $^{13}C_{60}$ I_h symmetry species:

A_g	9.6076798852693120000e+15
T_{1g}	2.8823036970926496000e+16
T_{3g}	2.8823036970926496000e+16
G_g	3.8430716856193728000e+16
H_g	4.8038396740938240000e+16

A_g	9.6076787936314240000e+15
T_{1g}	2.8823037990981216000e+16
T_{3g}	2.8823037990981216000e+16
G_g	3.8430716784610624000e+16
H_g	4.8038395577718272000e+16

Approximate species ratio: 1:3:3:4:5

Table 1. Frequency table relating the number of Y_h species { A_g, T_{1g}, T_{3g}, G_g, H_g, A_u, T_{1u}, T_{3u}, G_u, H_u } that correlate with each of the S_{60} permutation group species. The g and u characters in the parity column denote even and odd parity respectively, and the I column labels each of the pertinent S_{60} species by total nuclear spin.

W.G.Harter, D.E.Weeks, Chem. Phys. Letters 194,3(1992) pdf p.14

AMOP reference links on pages 2-4

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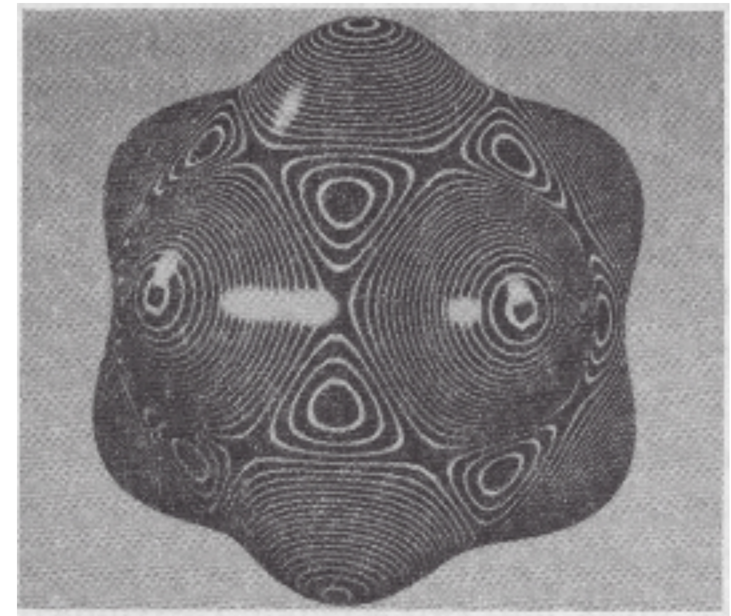
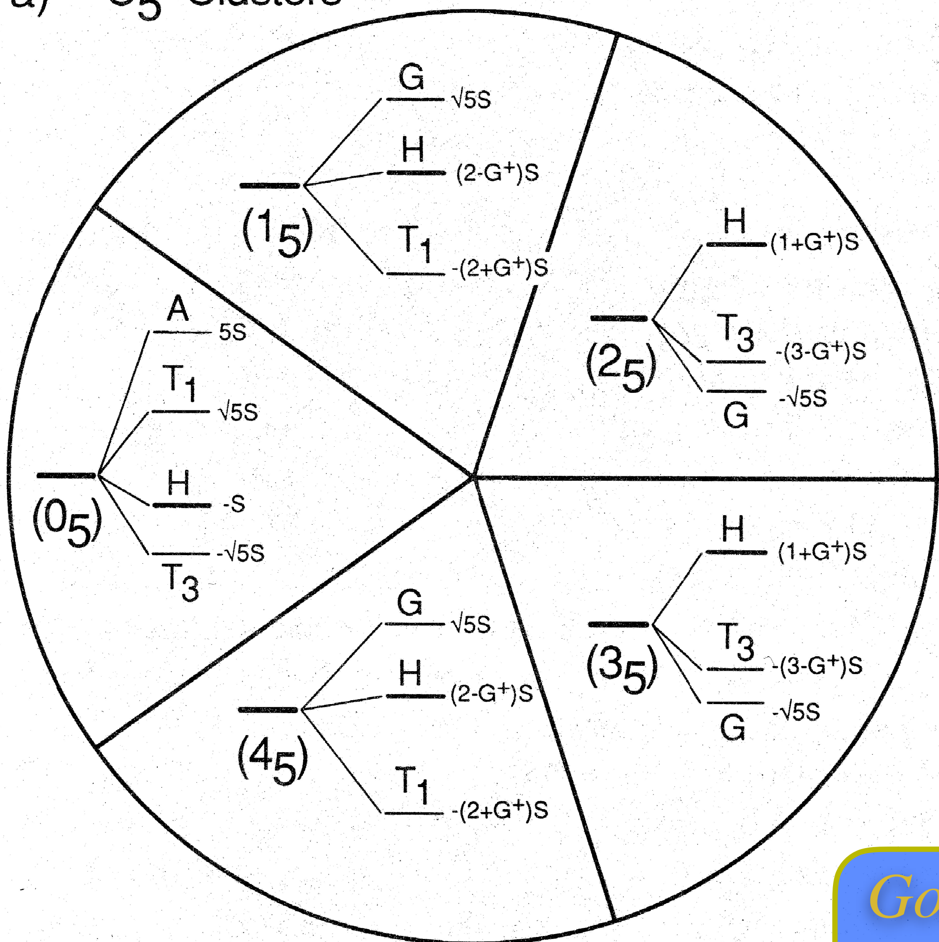
$^{13}C^{12}C_{59}$ isotopomers and their RES

Some history of C_{60} discoveries

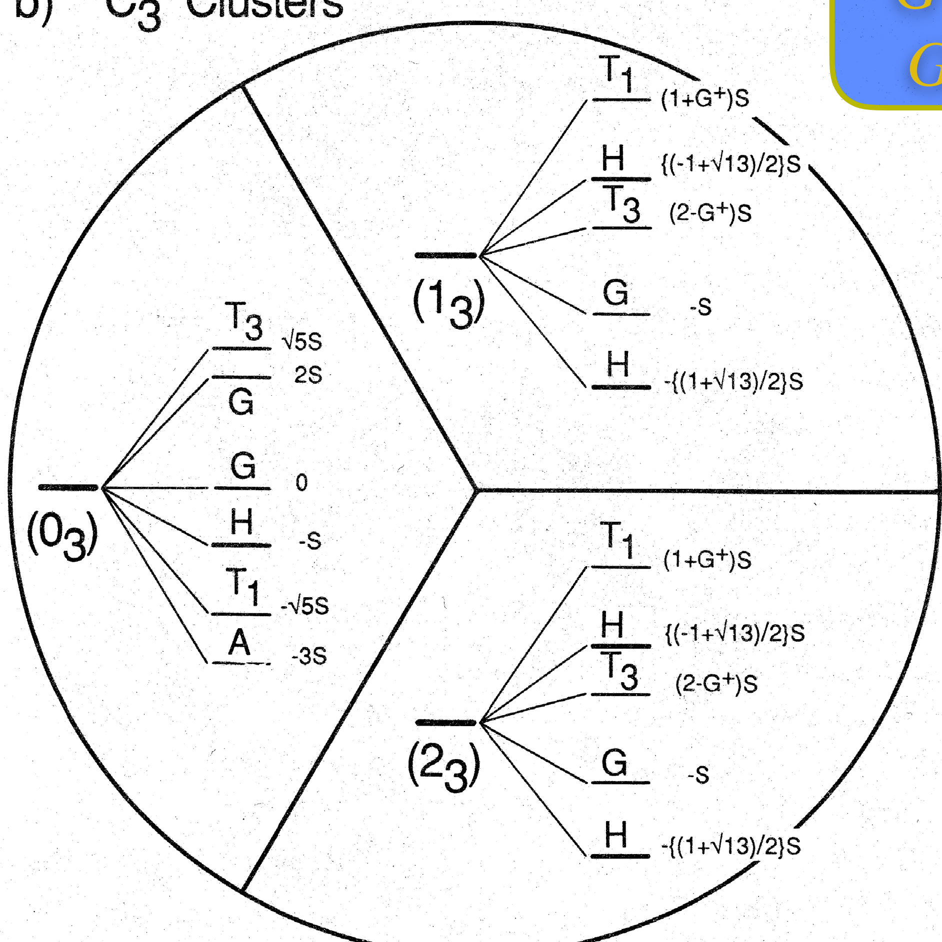
$^{13}C_{60}$ *superfine cluster structure predictions*



a) C_5 Clusters



b) C_3 Clusters

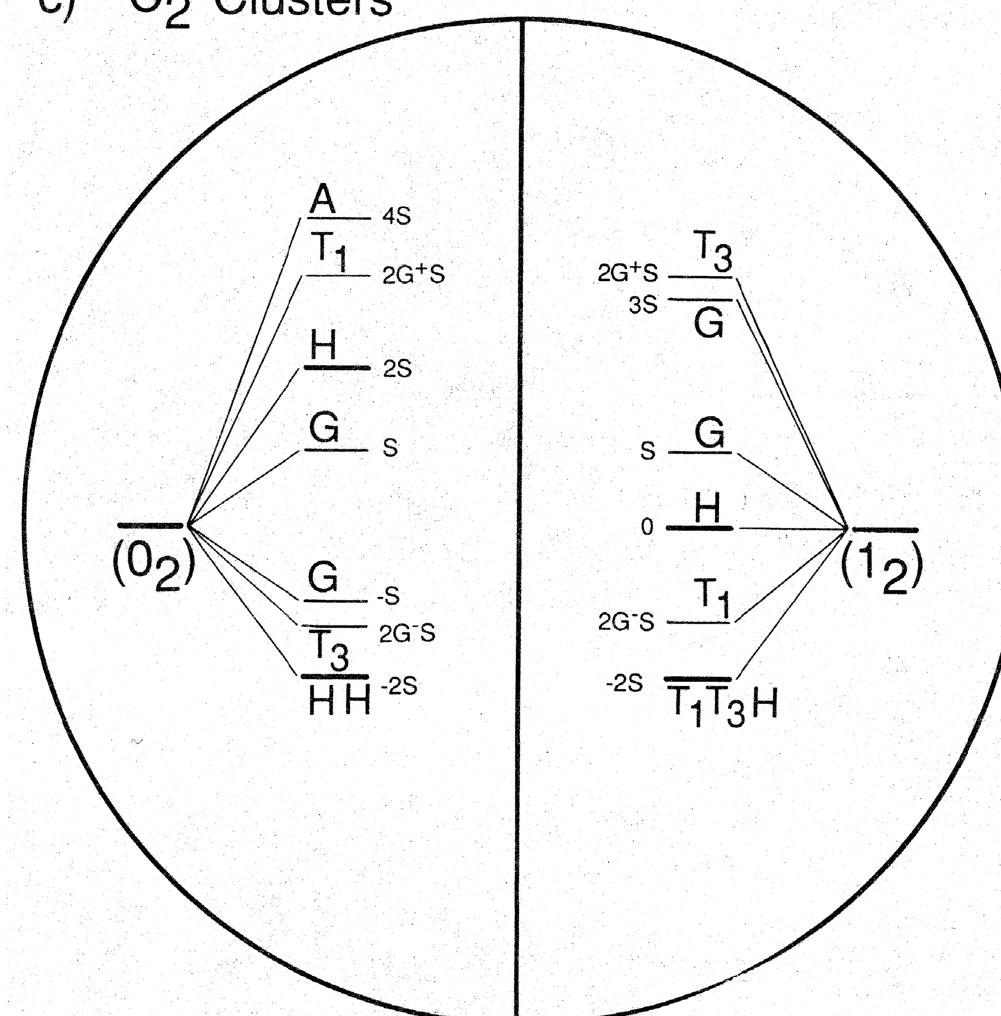


Golden Ratios

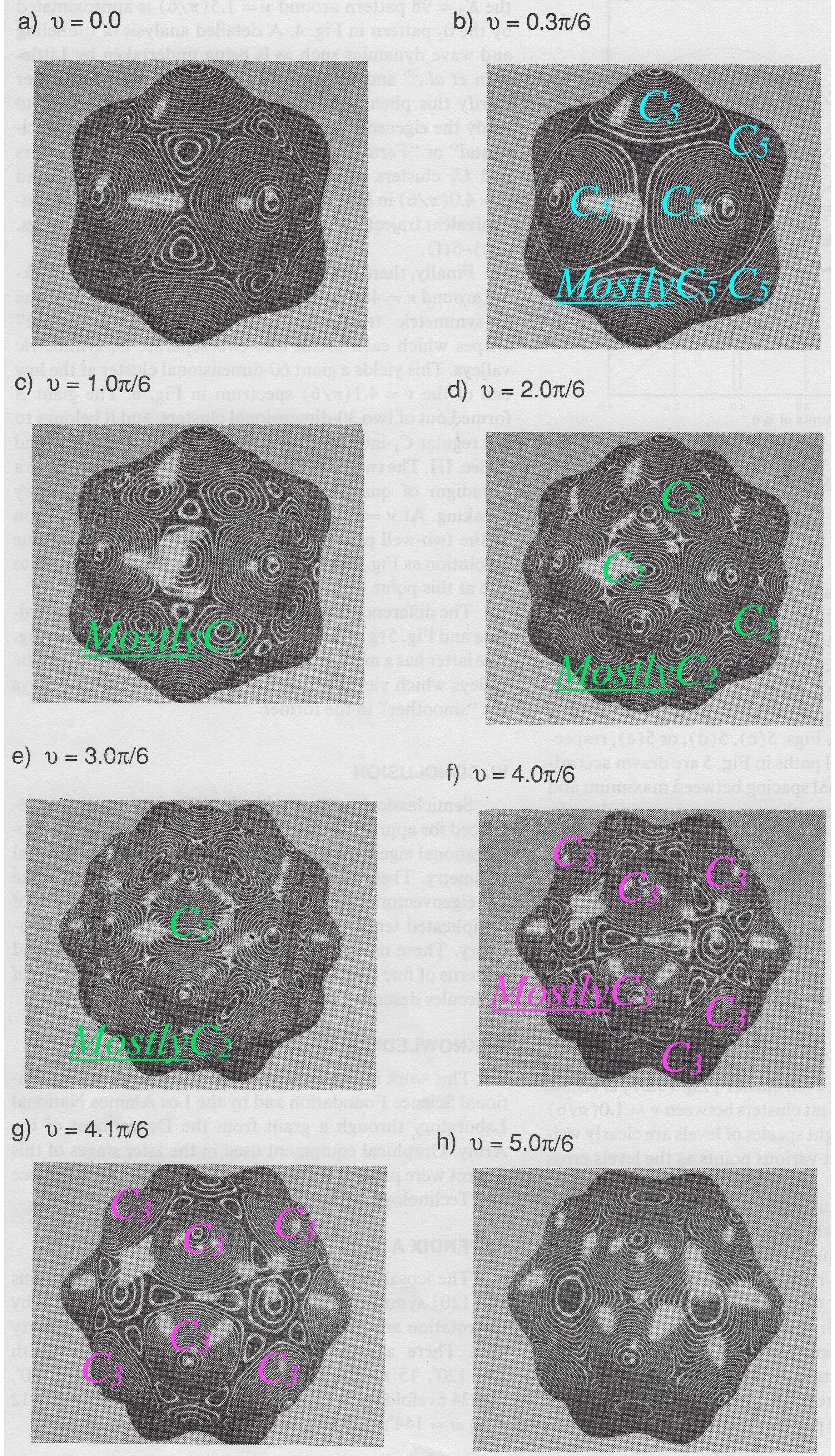
$G^{+}=(\sqrt{5}+1)/2 = 1.618\ldots$

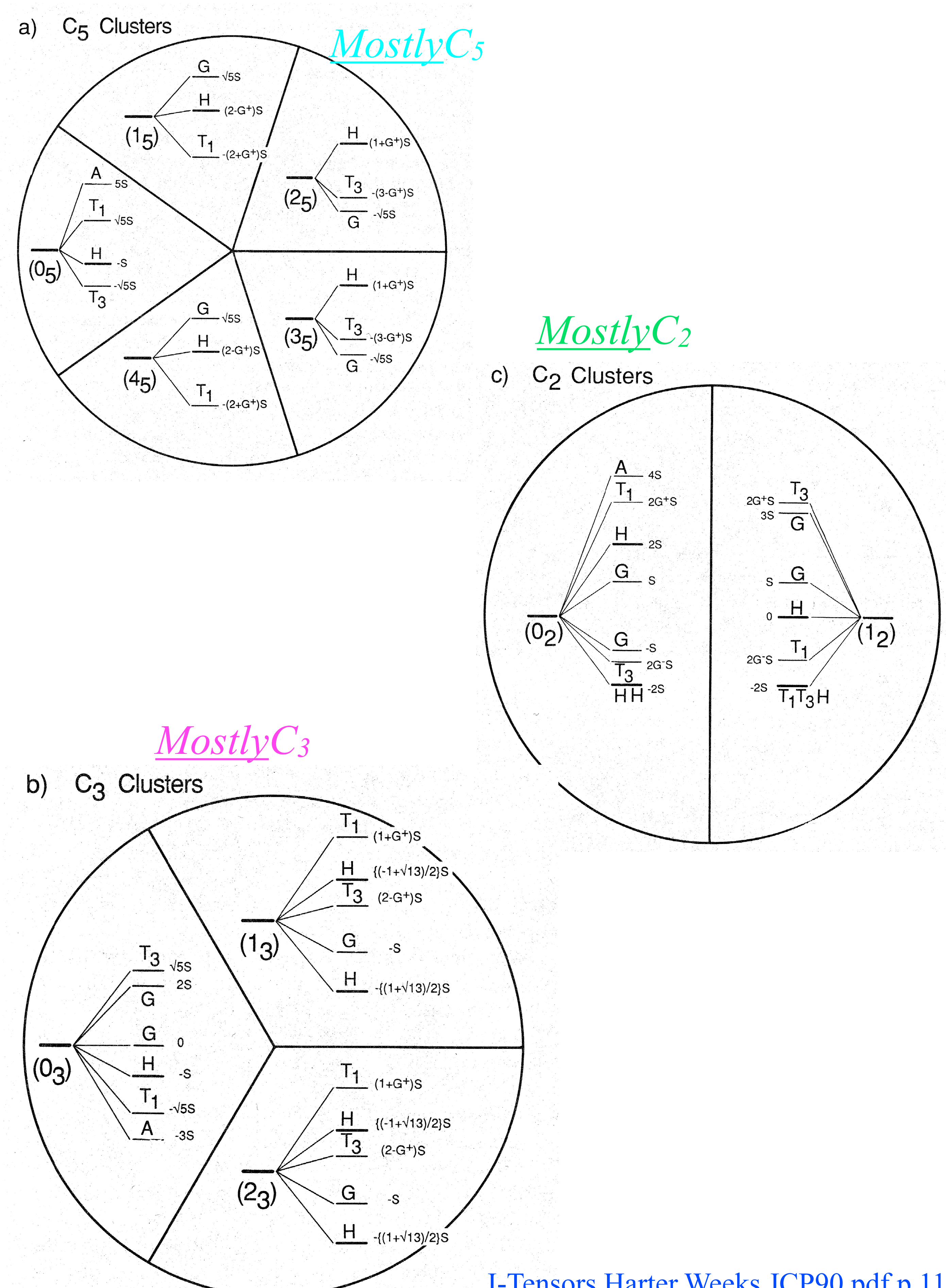
$G^{-}=(\sqrt{5}-1)/2 = 0.618\ldots$

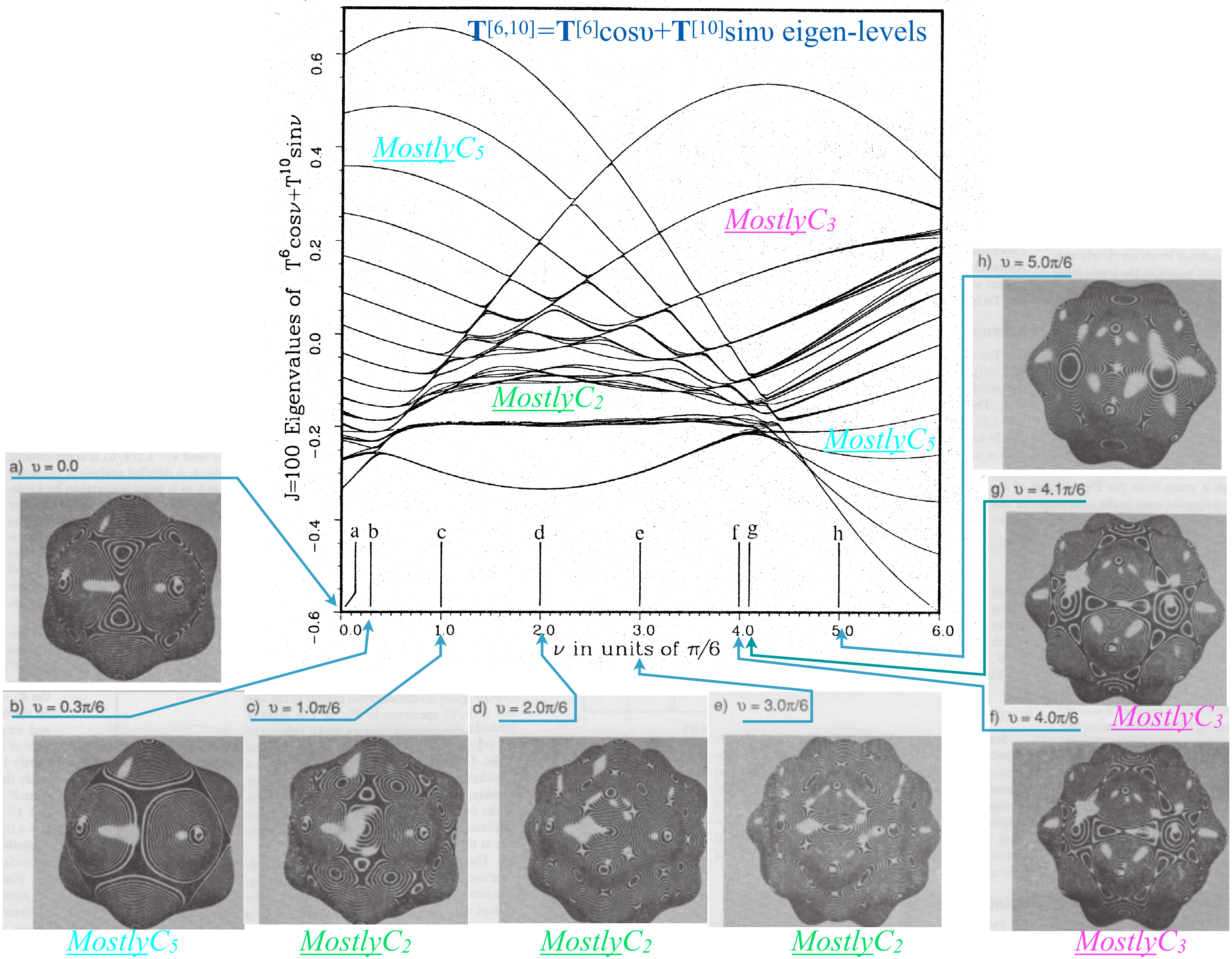
c) C_2 Clusters



$\mathbf{T}^{[6,10]}=\mathbf{T}^{[6]}\cos\upsilon+\mathbf{T}^{[10]}\sin\upsilon$ gives strange eigen-clusters







I-Tensors Harter,Weeks JCP90 pdf p.13

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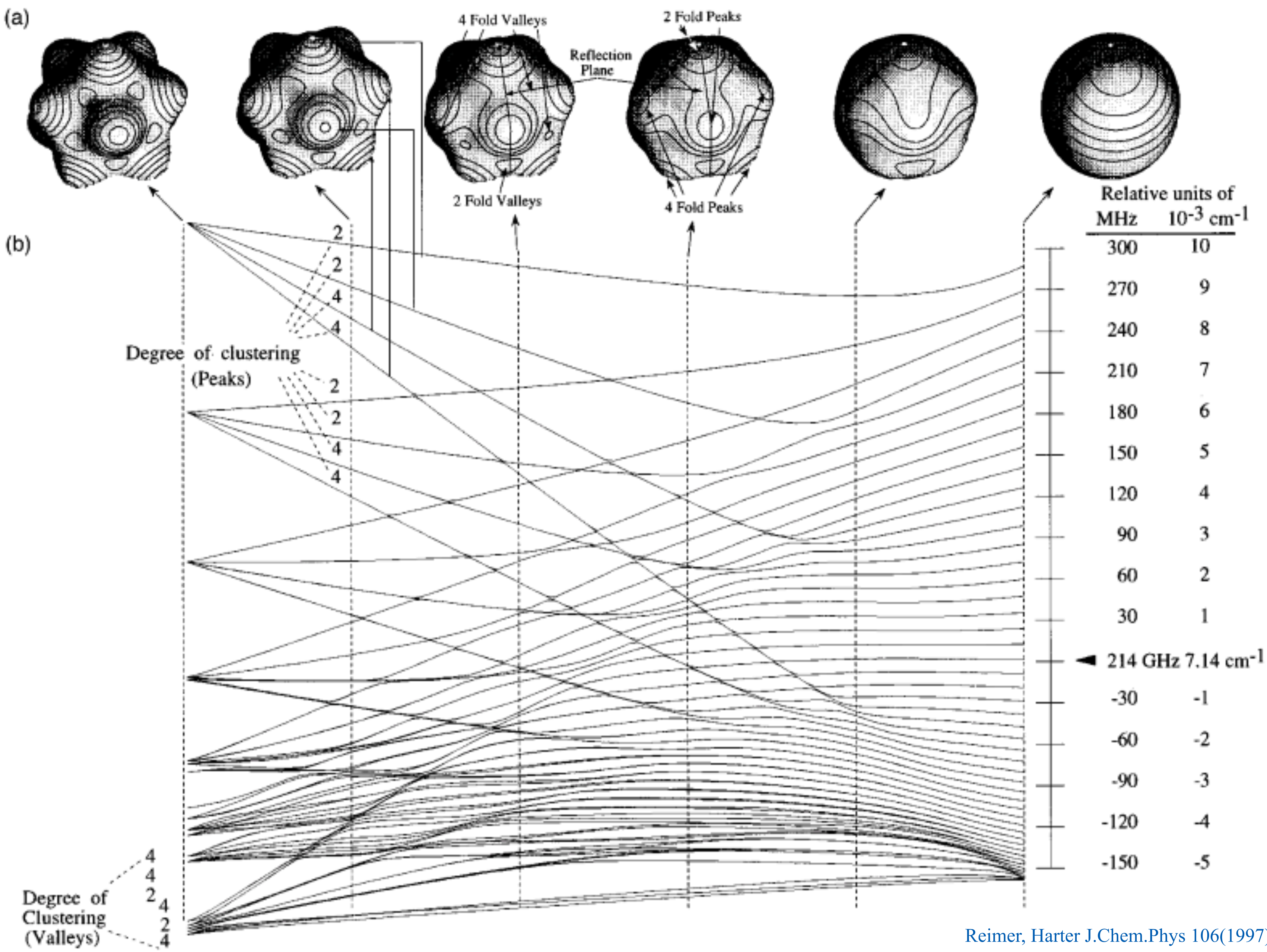
$^{13}C^{12}C_{59}$ isotopomers



Reimer, Harter J.Chem.Phys 106(1997) pdf p.5

FIG. 1. Rotational energy surfaces and ($J=50$) levels for Cs symmetry breaking. (a) Rotational energy surfaces varying from pure semirigid icosahedral (left) to pure symmetric top (right) molecules for $\tau=0,\frac{1}{5},..,1$. (b) Quantum mechanical energy levels for $|J|=50$ varied from pure semirigid icosahedral molecule (left) to purely rigid symmetric top perturbation. The energy scale on the right applies to rigid ^{13}C $^{12}C_{59}$ prolate top levels.

https://modphys.hosted.uark.edu/pdfs/Journal_Pdfs/C60symmReduct&fine%20structure12C13C59%20ReimerHarter1997hiRes.pdf#page=5

$^{13}C^{12}C_{59}$ isotopomers

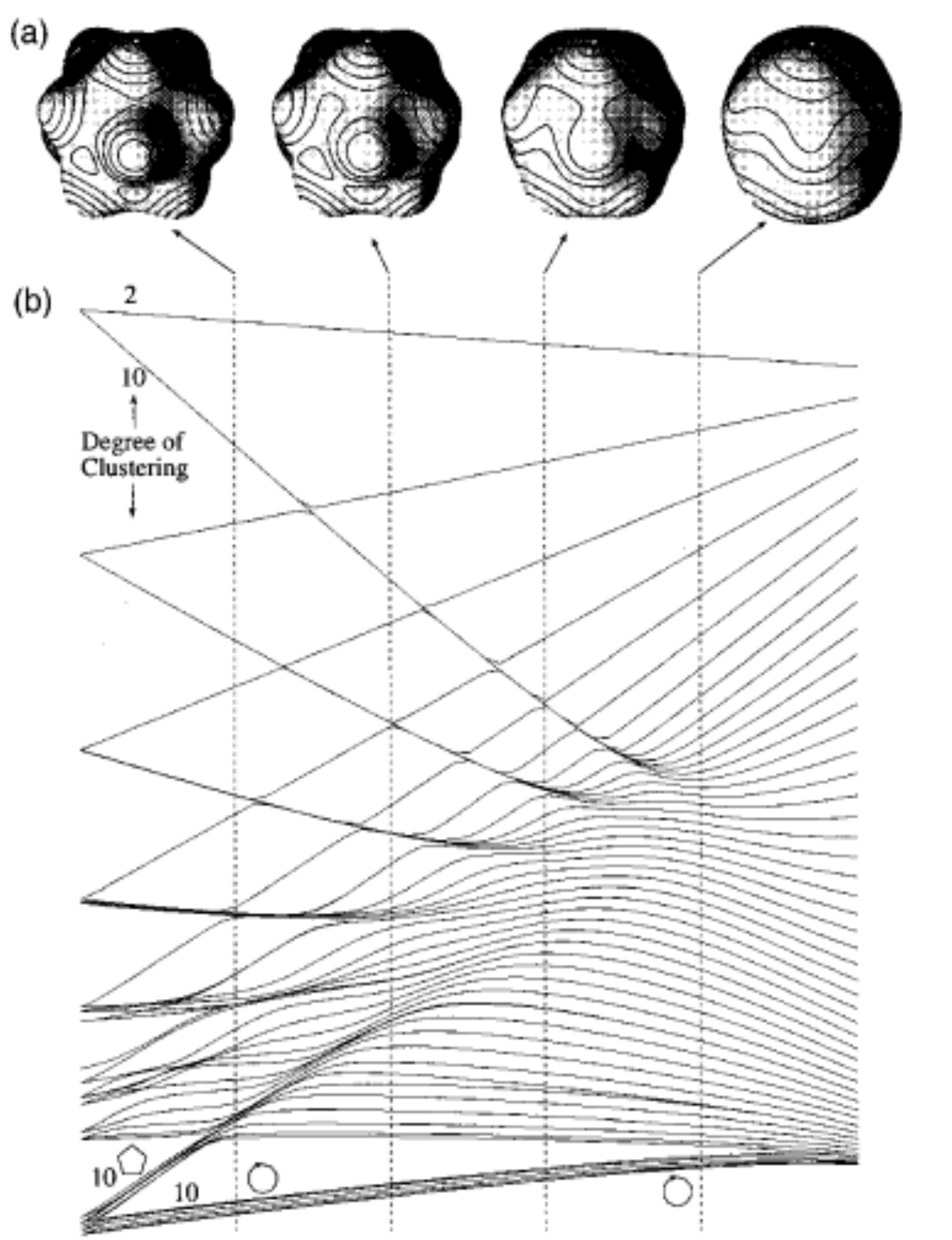


FIG. 3. Rotational energy surfaces and ($J=50$) levels for D_5-C_{5v} symmetry breaking. (a) Rotational energy surfaces varying from nearly icosahedral symmetry ($\tau=\frac{1}{5}$ on left) to nearly pure symmetric top ($\tau=\frac{4}{5}$ on right). (b) Quantum mechanical energy levels for $|J|=50$ varied from pure semirigid icosahedral molecule ($\tau=0$ on left) to pure symmetric top structure ($\tau=1$ on right) with dopant perturbation symmetry axis on a C_{5v} site.

Reimer, Harter J.Chem.Phys 106(1997) pdf p.7

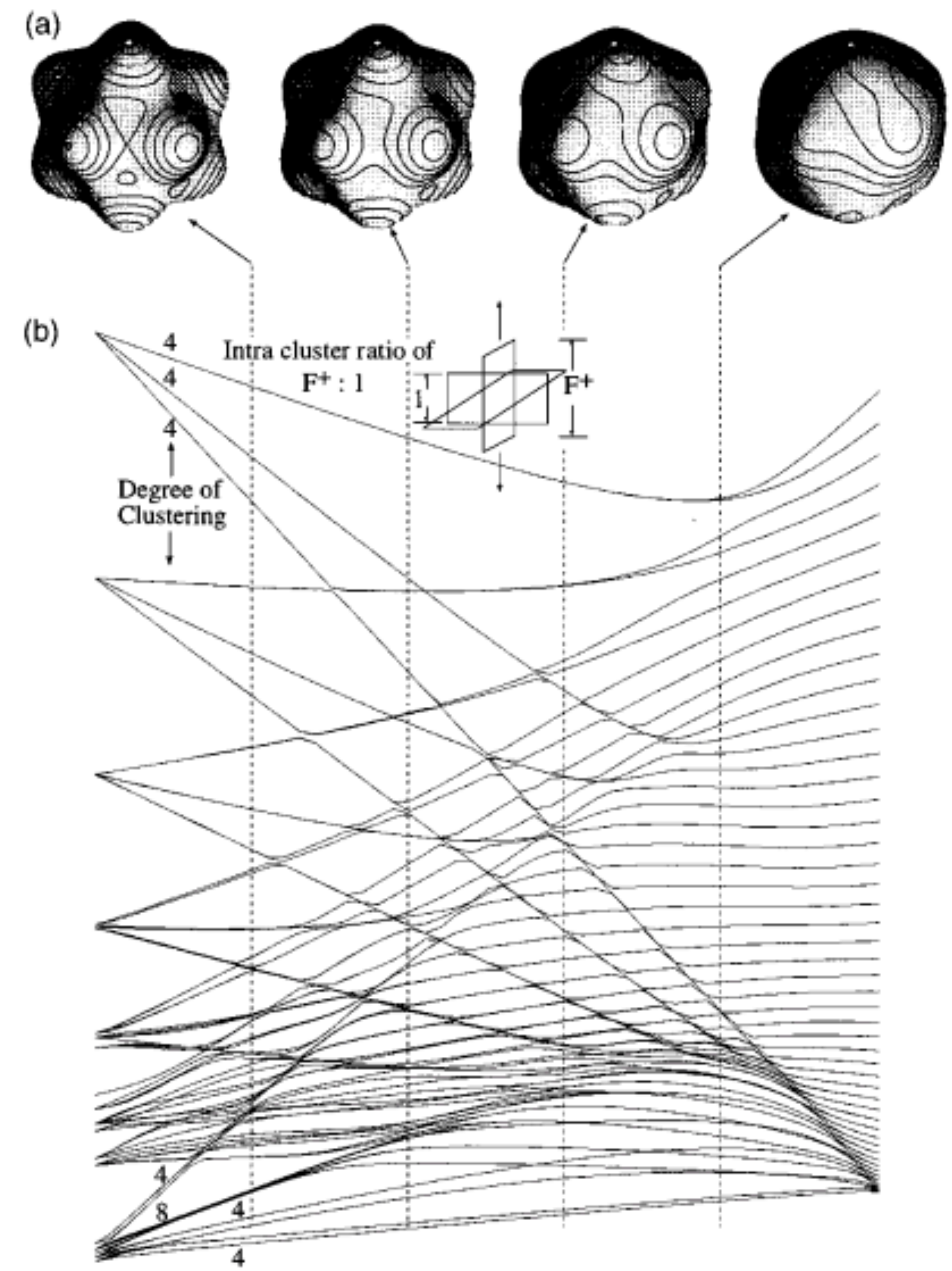


FIG. 5. Rotational energy surfaces and ($J=50$) levels for $C_{2h}-C_{2v}$ symmetry breaking. (a) Rotational energy surfaces varying from nearly icosahedral symmetry ($\tau=\frac{1}{5}$ on left) to nearly pure symmetric top ($\tau=\frac{4}{5}$ on right). (b) Quantum mechanical energy levels for $|J|=50$ varied from pure semirigid icosahedral molecule ($\tau=0$ on left) to pure symmetric top structure ($\tau=1$ on right) with dopant perturbation symmetry axis on a C_{2v} site.

https://modphys.hosted.uark.edu/pdfs/Journal_Pdfs/C60symmReduct&fine%20structure12C13C59%20ReimerHarter1997hiRes.pdf#page=7

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Buckyballs “Seen” in Space

A brief history of C_{60} spectroscopy

Bill Harter

UAF - Physics

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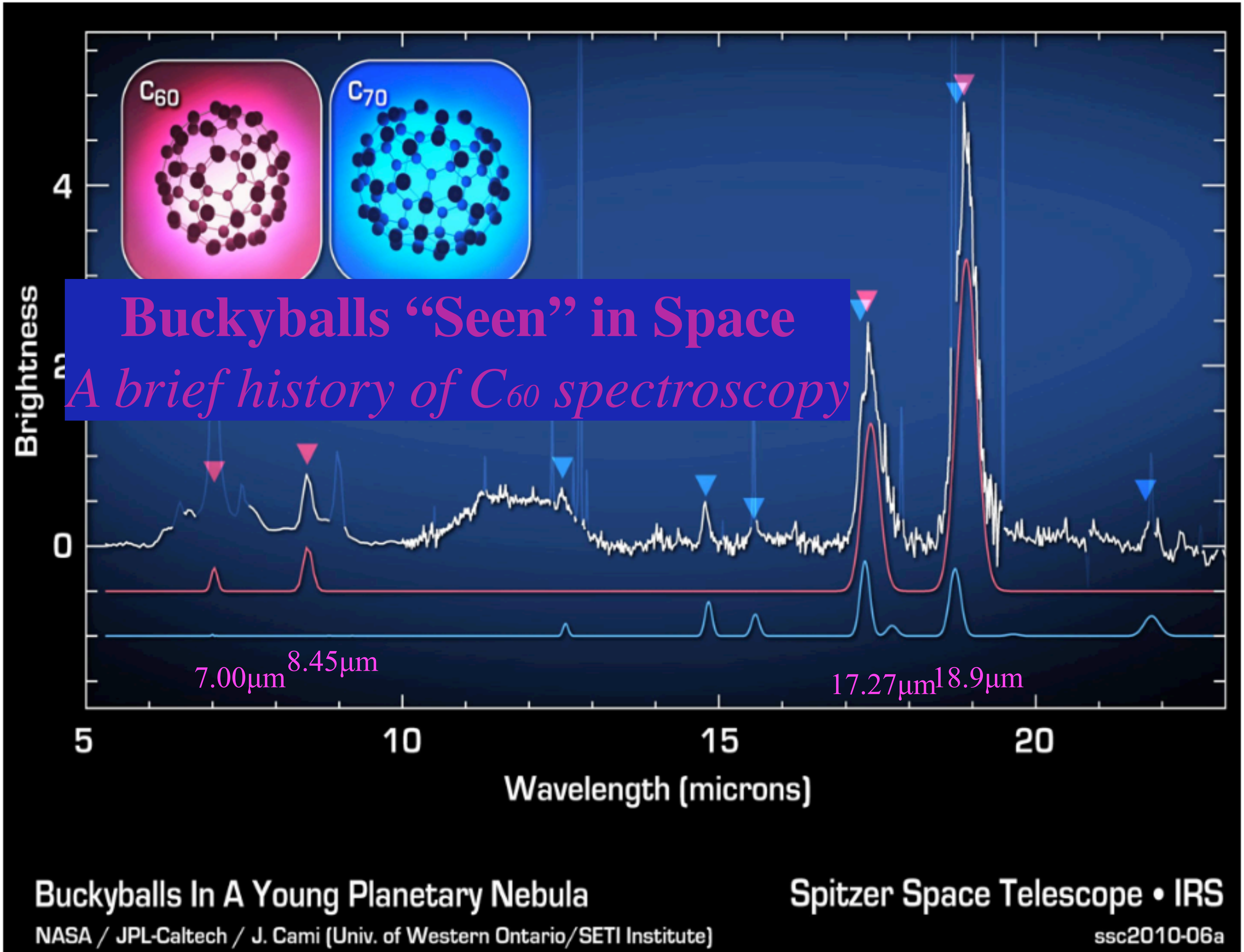


1st Try at "Seeing" in Lab

Mass spectroscopy gives something with atomic weight 720

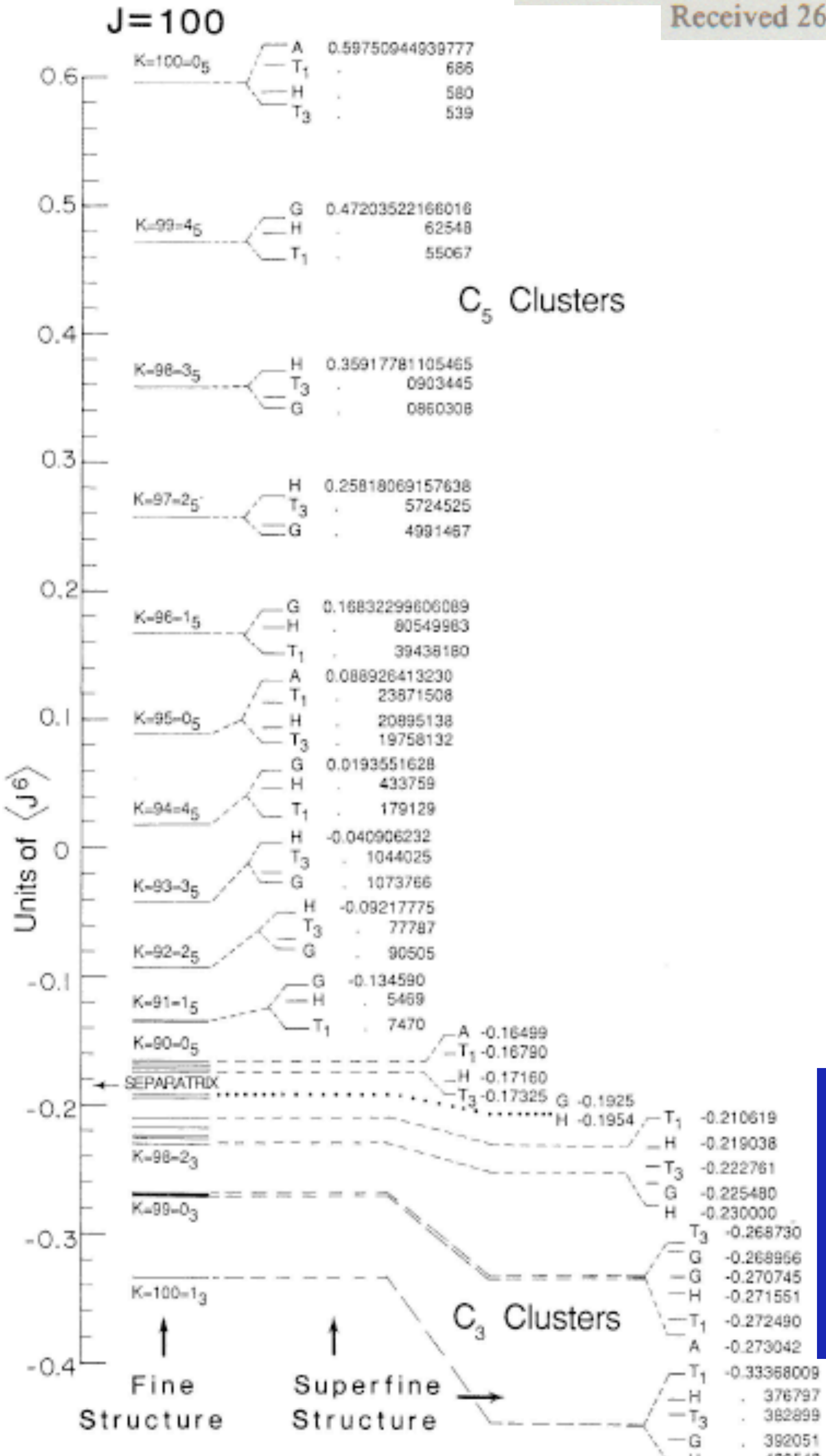
Richard Smalley, Bob Curl, and Harry Kroto (1985)
Guess structure is C_{60} "soccer ball"

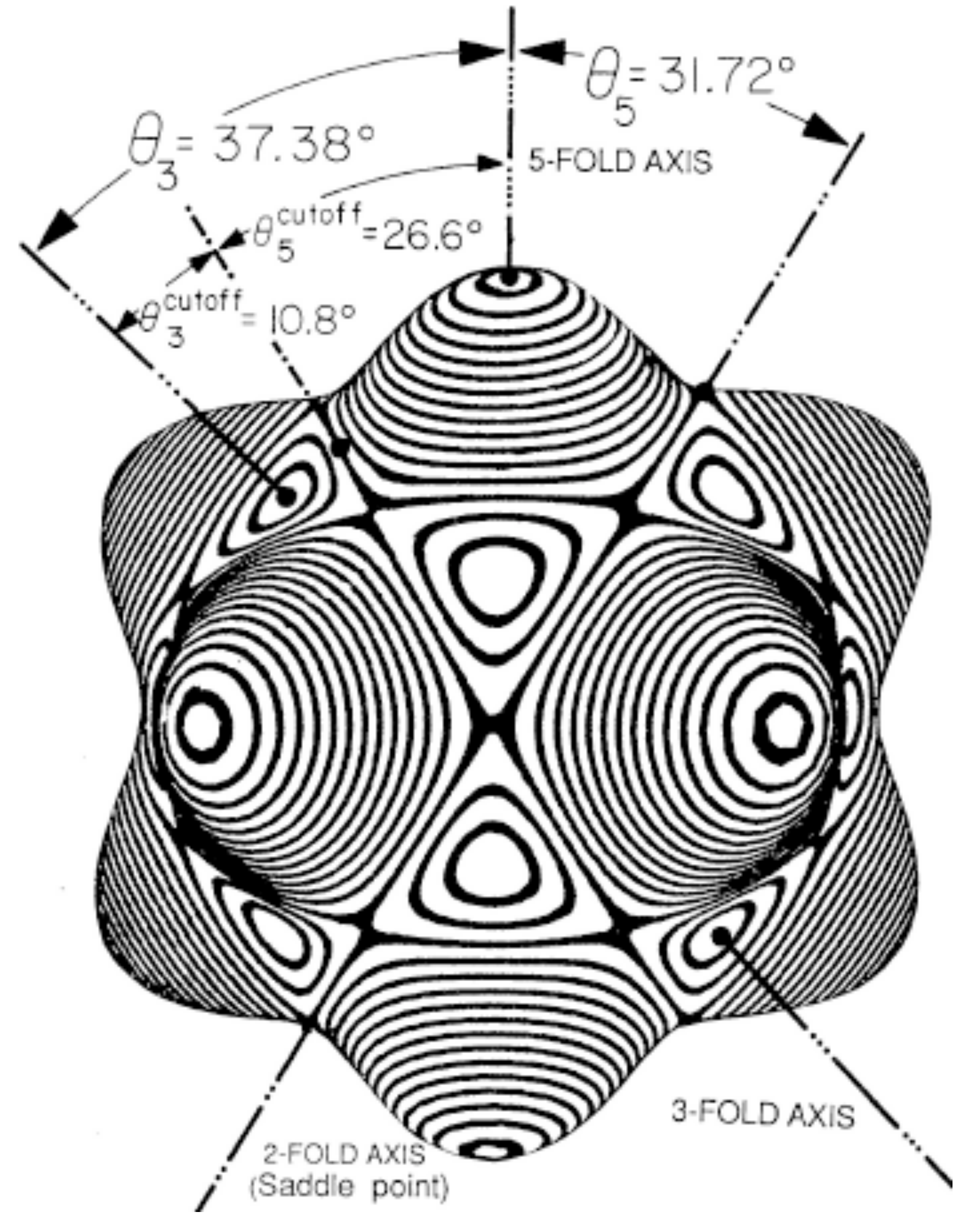
Volume 132, number 4,5 CHEMICAL PHYSICS LETTERS 19 December 1986

William G. HARTER and David E. WEEKS

Department of Physics, J. William Fulbright College, University of Arkansas, Fayetteville, AR 72701, USA

Received 26 August 1986





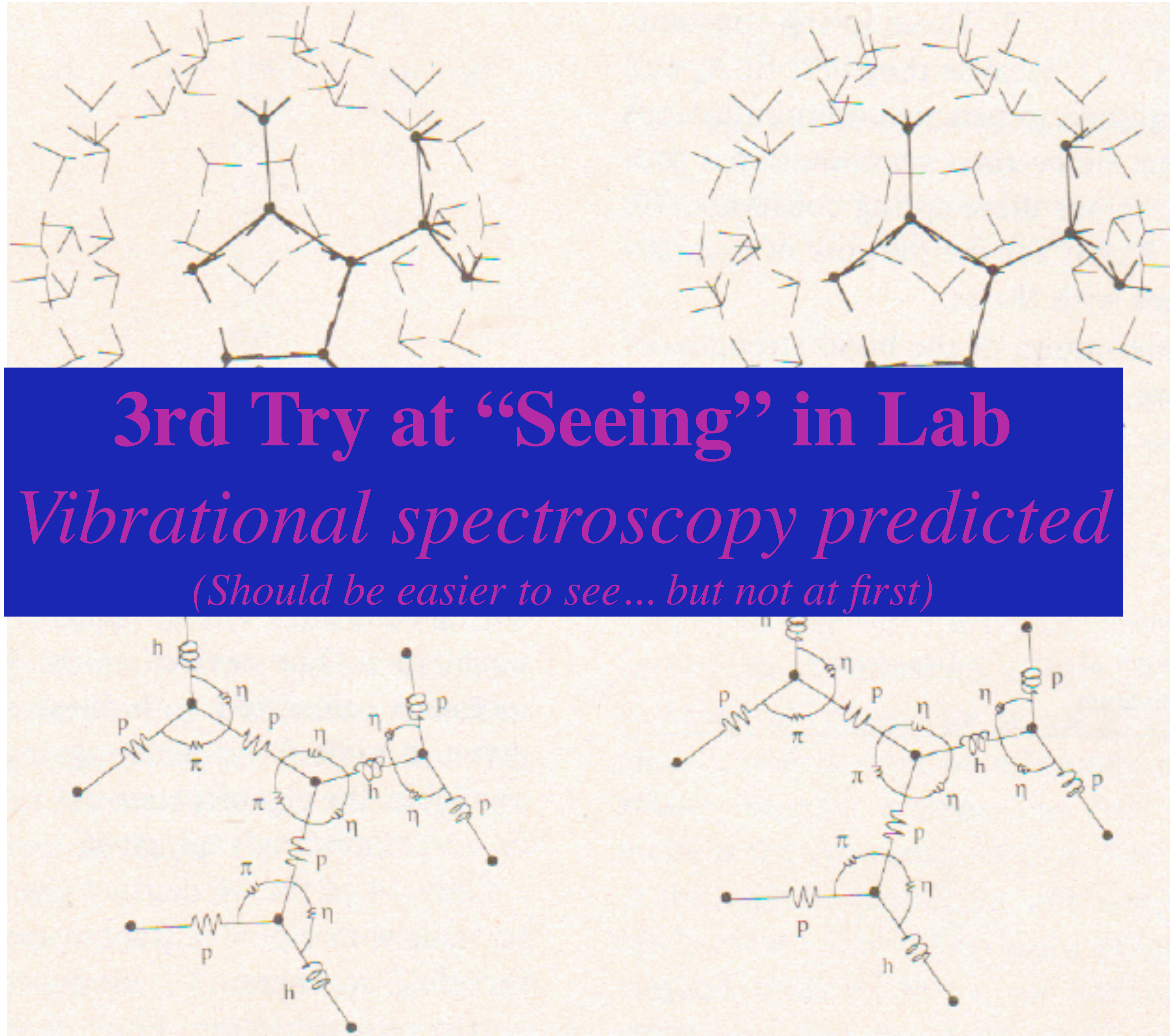
2nd Try at "Seeing" in Lab

Rotational spectroscopy predicted

(but still too hard to see)

3·60=180 coordinates of C_{60}

"Buckyball" vibrational coordinates



3rd Try at "Seeing" in Lab

Vibrational spectroscopy predicted

(Should be easier to see… but not at first)

Volume 144, number 4 CHEMICAL PHYSICS LETTERS 4 March 1988

VIBRATIONAL FREQUENCIES AND NORMAL MODES OF BUCKMINSTERFULLERENE

David E. WEEKS and William G. HARTER

3rd Try(contd)

Vibration spectra predicted (Easy to see… just 2 pairs of lines)

Volume 144, number 4 CHEMICAL PHYSICS LETTERS 4 March 1988

Table 3
Symmetry-labeled eigenfrequencies of Buckyball for $p=h=7.6\times10^5$ dyn/cm, $\pi=\eta=0.7\times10^5$ dyn/cm

Even parity		Odd parity	
I_h group label	frequency (cm^{-1})	I_h group label	frequency (cm^{-1})
A_g	1830	A_u	1243
	510		
T_{1g}	1662	T_{1u}	1868
	1045		1462
	513		618
			478
T_{3g}	1900	T_{3u}	1954
	951		1543
	724		1122
	615		526
			358
G_g	2006	G_u	2004
	1813		1845
	1327		1086
	657		876
	593		663
	433		360
H_g	2068	H_u	2086
	1910		1797
	1575		1464
	1292		849
	828		569
	526		470
	413		405
	274		

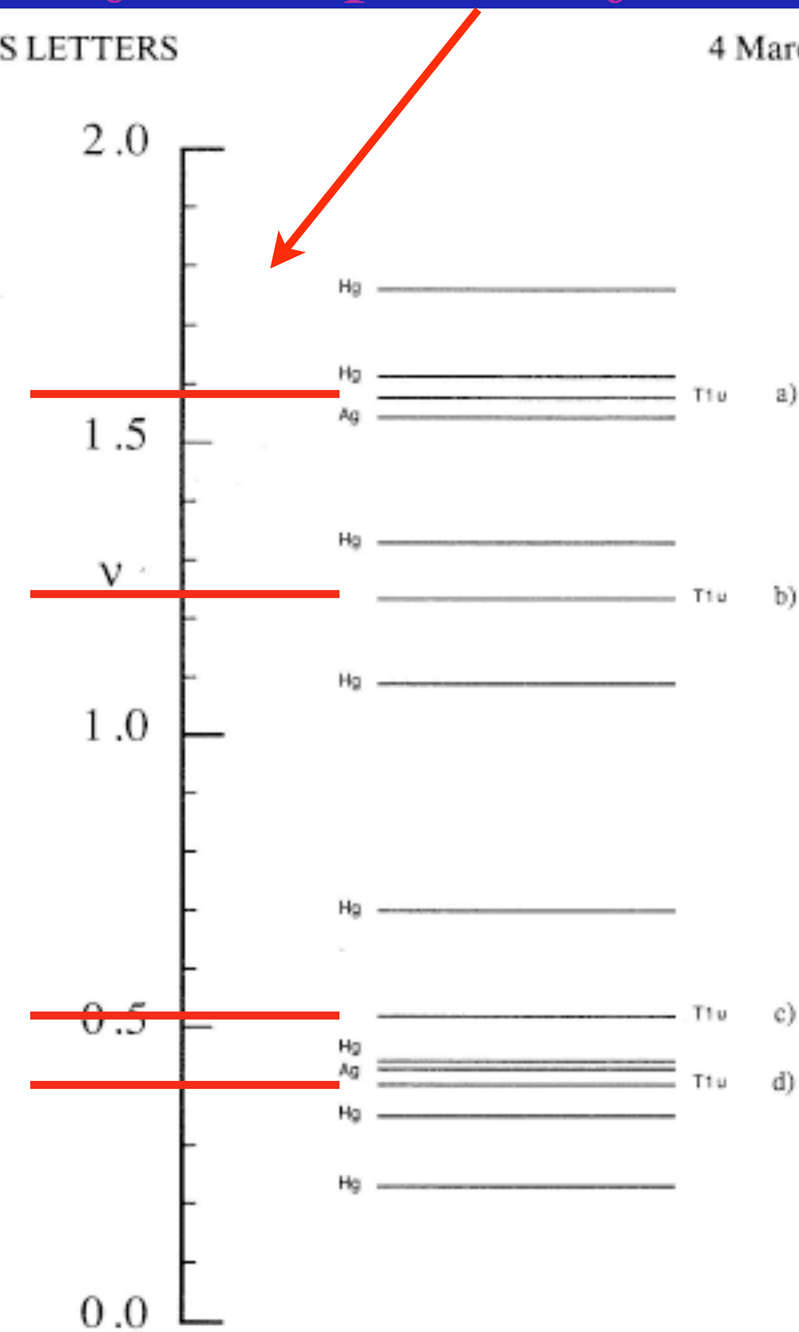
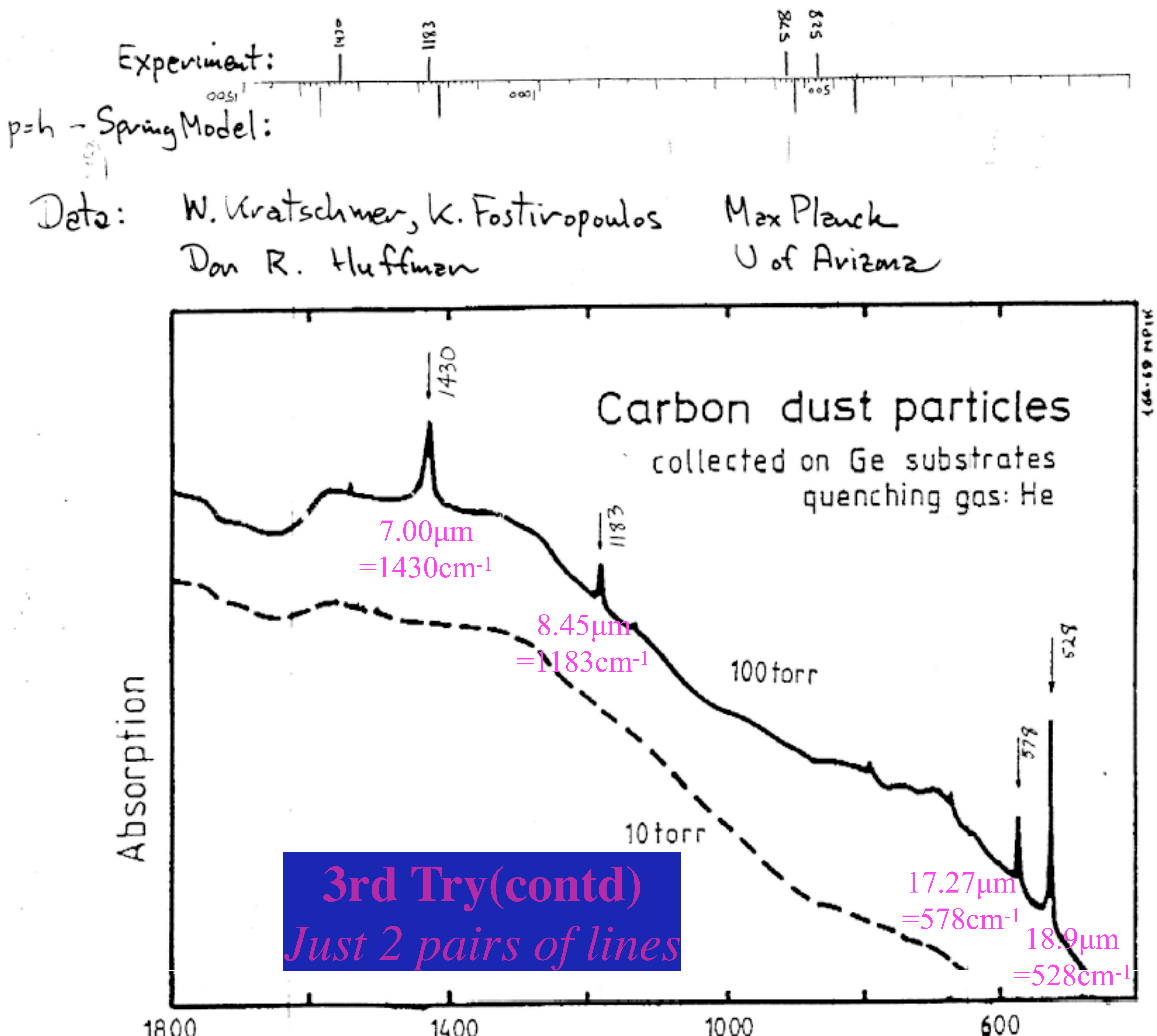
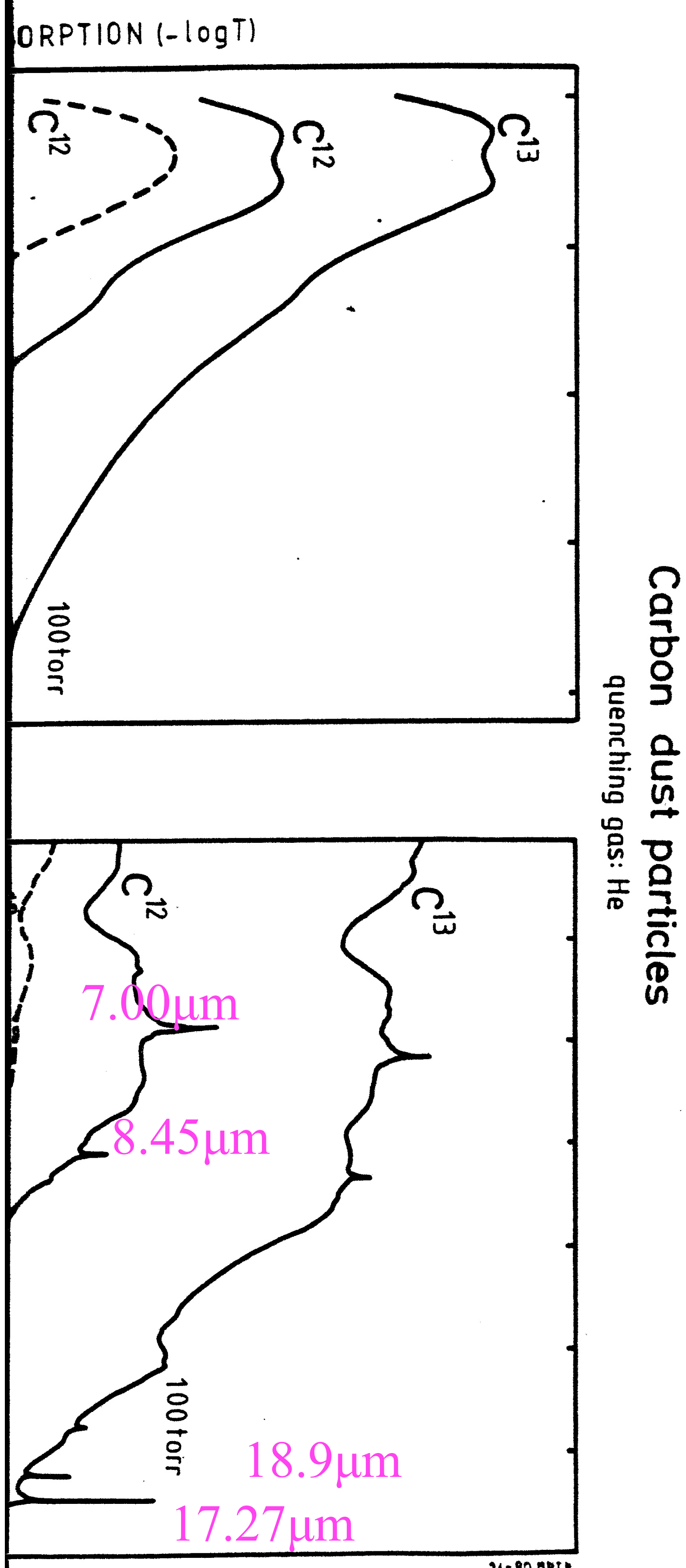


Fig. 3. Spectrum of the possibly dipole and Raman active modes of Buckyball. The spring constants are $p=h=7.6\times10^5$ dyn/cm and $\pi=\eta=0.7\times10^5$ dyn/cm. The scale is in units of 1185 cm^{-1}. Lines a–d correlate with eigenmodes in fig. 4.


Experiment:
1430
1183
578
528
p=h - Spring Model:
Data: W. Kratschmer, K. Fostiropoulos Max Planck
Don R. Huffman U of Arizona
Carbon dust particles
collected on Ge substrates
quenching gas: He
Absorption
7.00μm
=1430cm-1
8.45μm
=1183cm-1
100 torr
10 torr
529
579
17.27μm
=578cm-1
18.9μm
=528cm-1
3rd Try(contd)
Just 2 pairs of lines
1800
1400
1000
600



THE UNIVERSITY OF ARIZONA
TUCSON, ARIZONA 85721 USA

COLLEGE OF ARTS AND SCIENCES
FACULTY OF SCIENCE
DEPARTMENT OF PHYSICS
BUILDING #81
(602) 621-6820

May 23, 1990

Dr. William G. Harter
Dept. of Physics
The University of Arkansas
Fayetteville, Arkansas 72701

Dear Bill,

Here is a copy of the first paper on C_{60} which has just been accepted for publication in Chem. Phys. Letters.

We have had much fun with your program. It is delightful.

Things are moving very fast in the Buckyball arena. We now think we can concentrate the material and produce it in sufficient quantity for many experiments.

Thanks again for the discussions we have had and for your program.

Sincerely,

Dan

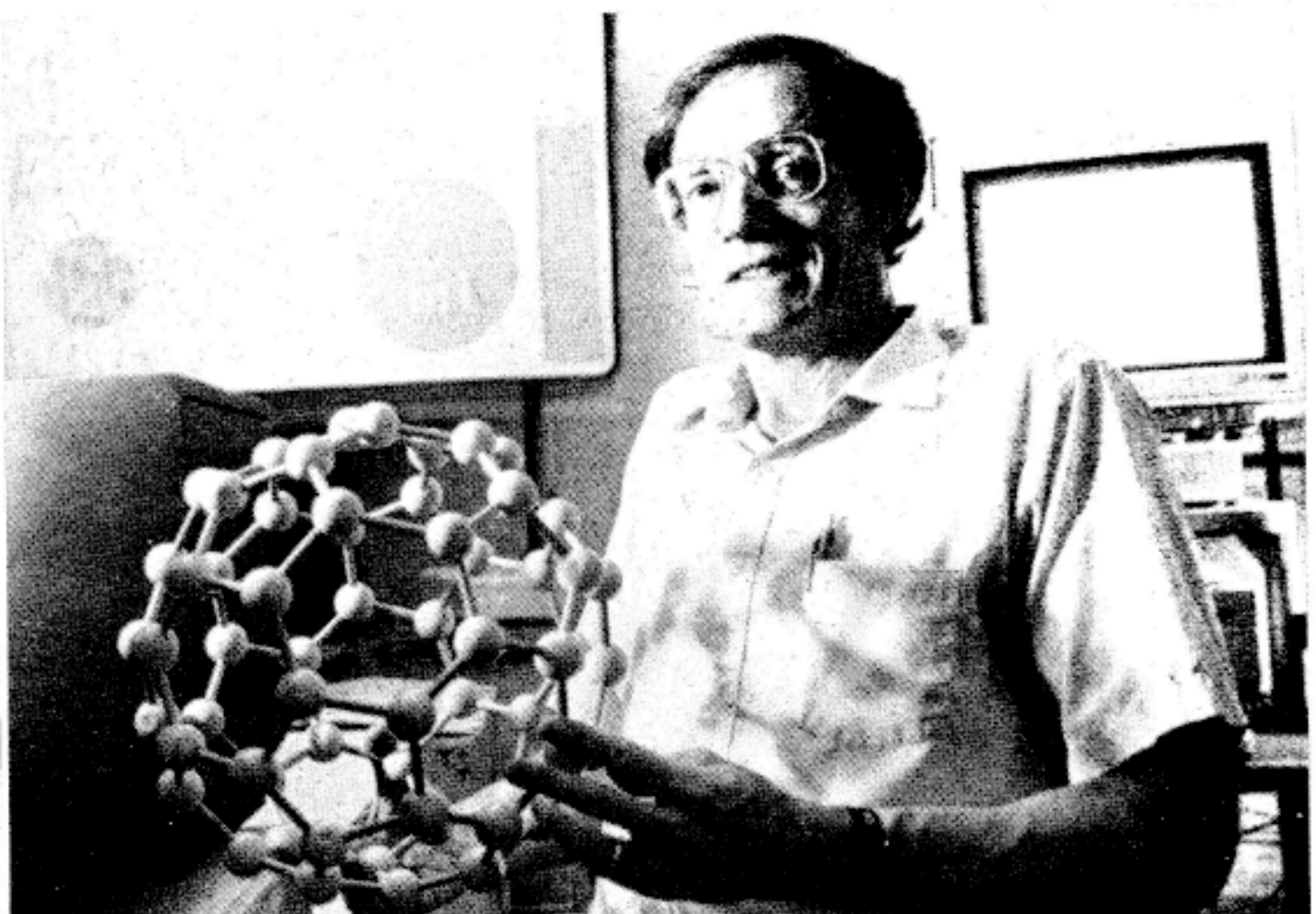
Donald R. Huffman
Professor of physics

DRH
Incl.

Fig 12.4.2

a tunable laser and discovered that molecular rotation resembles just what its name implies—the rotation of a planet on its axis. As molecules spin around their center of gravity, they wobble in a conical pattern or "precess" as they rotate around a multitude of axes. Also, molecules execute a generally slower "tunneling" or tumbling motion that would be forbidden in a world

Former Georgia Tech physics professor Dr. William Harter proposed a molecular rotational dynamics theory he used to make the first predictions on the rotational-vibrational spectra of the soccer ball-shaped molecule Buckminsterfullerene (C60), nicknamed "buckyball."



Physicist William Harter has come up with innovative teaching solutions to help reduce the 'physics anxiety' of students faced with galloping light waves, quantum mechanics, and the paradoxes of the physical universe. (Photo by Marc Francoeur)

spectra of the soccer ball-shaped molecule Buckminsterfullerene (C60), nicknamed "buckyball."

This structure had been proposed in 1985 by a group of Rice University researchers, who had seen a mass-spectra peak of atomic mass 720. Subsequently, researchers from the University of Arizona and the Max Planck Institute used Harter and Weeks' findings and their Macintosh software program to further analyze C60.

In 1989, those researchers realized from Harter and Weeks' vibrational spectral predictions that they had been making C60 since the early 1970s. Other experts were skeptical, but IBM labs at San Jose, Calif. verified the University of Arizona's results in 1990. Just two years later, *Science* named C60 "Molecule of the Year," and the Rice University-led research team received a Nobel Prize in chemistry in 1996 for its work with the molecule.

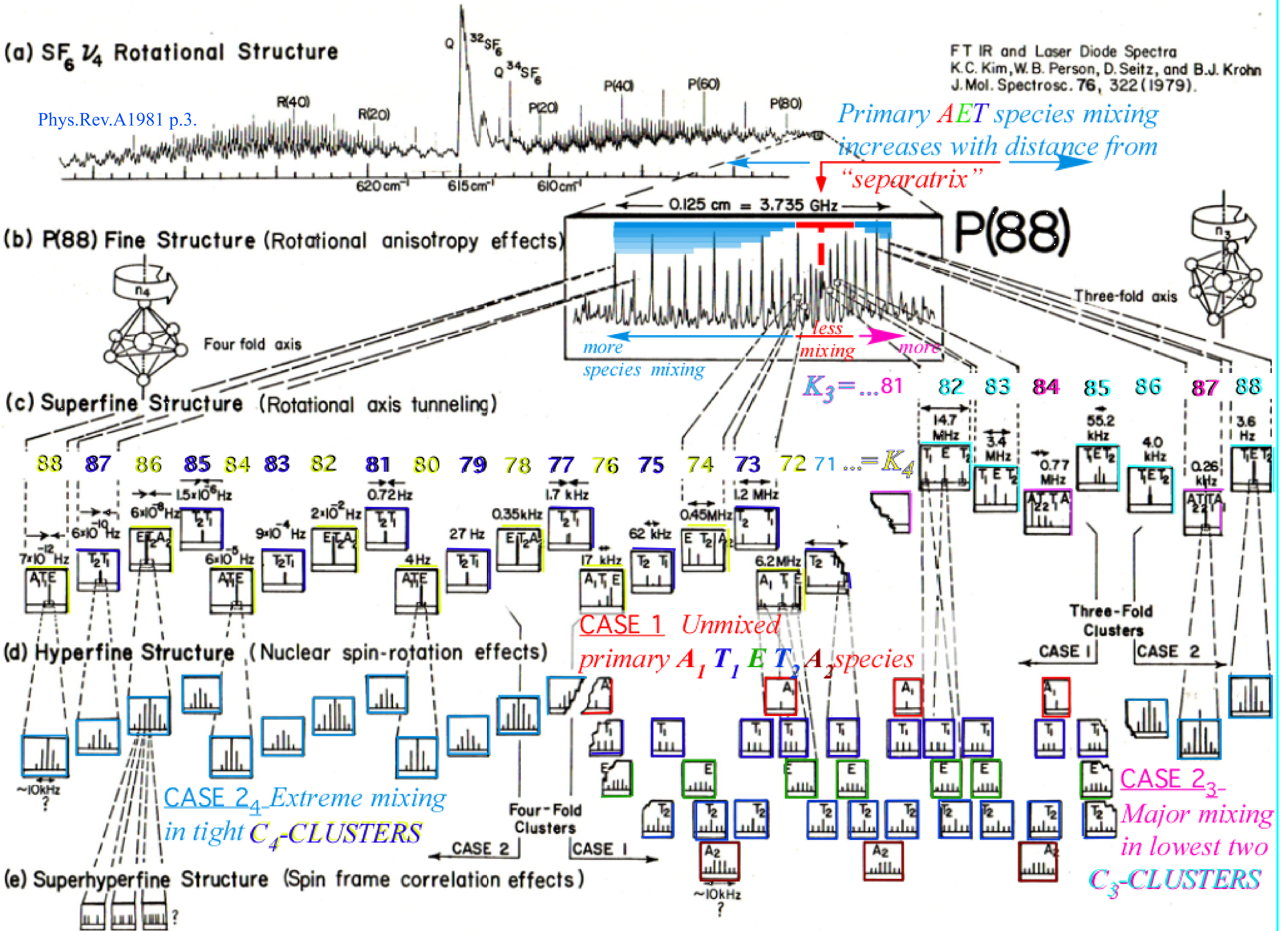
Harter is now a professor of physics at the University of Arkansas, where he studies optimal control theory for quantum systems. In 1995, he was elected a fellow of the American Physical Society. Weeks is a professor at the U.S. Air Force Postgraduate School near Wright Patterson AFB in Dayton, Ohio.

■ For more information, contact Dr. William Harter at wharter@comp.uark.edu.

Two (or Three) forms of Carbon on one license plate!

Here is a link to the new scenario at: https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=OhXY6

May Buckylamp light
your way always!



(a) SF6 ν4 Rotational Structure
Phys.Rev.A1981 p.3.
Q 32SF6
Q 34SF6
R(40)
R(20)
P(20)
P(40)
P(60)
P(80)
620 cm-1
615 cm-1
610 cm-1
FT IR and Laser Diode Spectra
K.C. Kim, W.B. Person, D. Seitz, and B.J. Krohn
J. Mol. Spectrosc. 76, 322 (1979).
Primary AET species mixing
increases with distance from
"separatrix"
0.125 cm = 3.735 GHz
P(88)
(b) P(88) Fine Structure (Rotational anisotropy effects)
Four fold axis
Three-fold axis
more
species mixing
less
mixing
more
K3 = ...81 82 83 84 85 86 87 88
(c) Superfine Structure (Rotational axis tunneling)
88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 ... = K4
CASE 1 Unmixed
primary A1 T1 E T2 A2 species
Three-Fold
Clusters
CASE 1
CASE 2
(d) Hyperfine Structure (Nuclear spin-rotation effects)
CASE 24 Extreme mixing
in tight C4-CLUSTERS
Four-Fold
Clusters
CASE 2
CASE 1
CASE 23-
Major mixing
in lowest two
C3-CLUSTERS
(e) Superhyperfine Structure (Spin frame correlation effects)