Heegaard Splitting of Critical Nets on Orbifolds

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What is a Critical Net? — A way of summarizing the relevant topological features into a single graph. Simply represent each atom by its thermal-motion density and then find the critical points and their topological connections.

Minimum gradient:

$$\text{Peak} \rightarrow \text{Pass} \rightarrow \text{Pale} \rightarrow \text{Pit}$$

Maximum gradient:

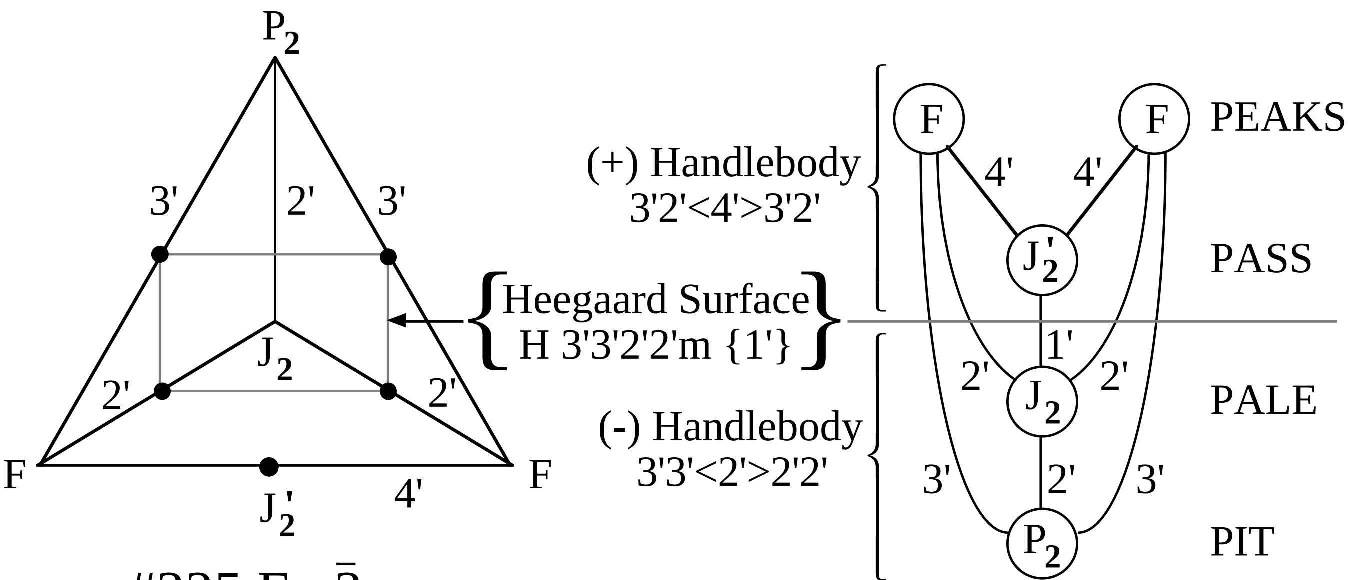
$$\text{Peak} \rightarrow \text{Pit}$$

What is an Orbifold? — A way to eliminate symmetry repetition. Simply divide Euclidean 3-space by the space group symmetry to obtain a wrapped-up asymmetric unit without discontinuities. The geometric symmetry elements appear as a singular-set graph in the orbifold. Critical nets may be superimposed onto orbifolds.

What is Heegaard Splitting? — A Heegaard surface separates the peaks + passes from the pales + pits. It splits the orbifold into a pair of handlebody orbifolds.

Example Heegaard Splitting of Orbifold

Orbifold (left) and critical net on orbifold (right). The Heegaard surface is a 2-orbifold joining two handlebody 3-orbifolds to form the Euclidean 3-orbifold.

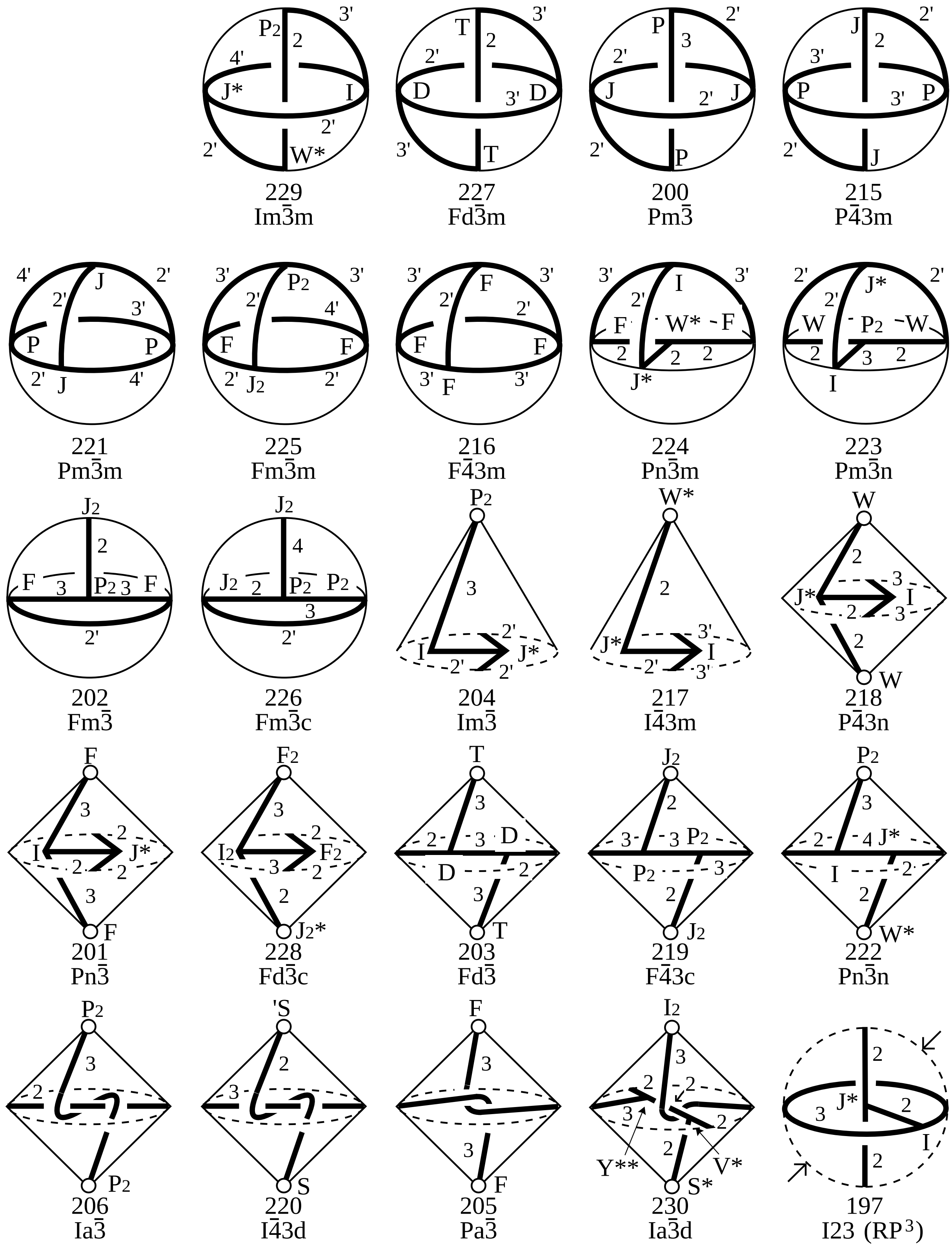


#225 $Fm\bar{3}m$

This 3-orbifold is bounded by the mirror faces of the $Fm\bar{3}m$ tetrahedral asymmetric unit. Symbols and integers denote invariant lattice complex sites and symmetry axes numbers, respectively.

NaCl critical net on $Fm\bar{3}m$ orbifold with circled critical points on sites F,F/J2'/J2/P2. Na and Cl are on the two F critical point sites.

The 24 Cubic Orbifolds that Do Not Have S^3 as an Underlying Space

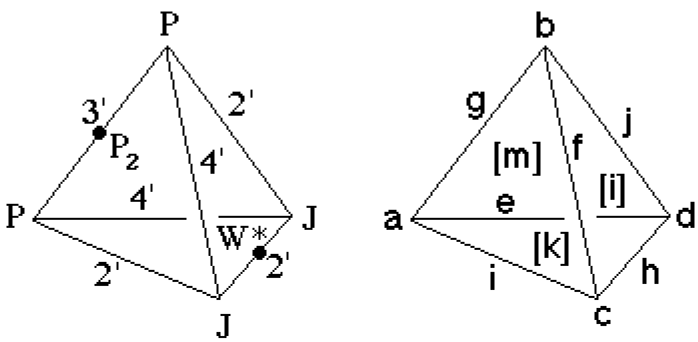


Tetrahedral Euclidean 3-Orbifolds

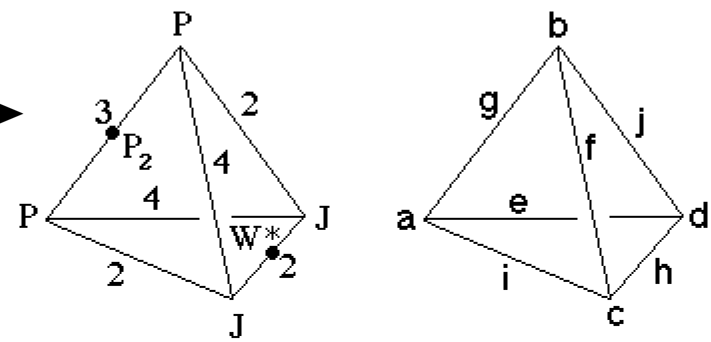
Left figure - axis-order integers (primed if on mirror) and lattice complex symbols. Right figure - Wyckoff site letters in [ ] if mirrors. Arrow denotes index-2 subgroup.

<u>Underlying Space D^3</u>

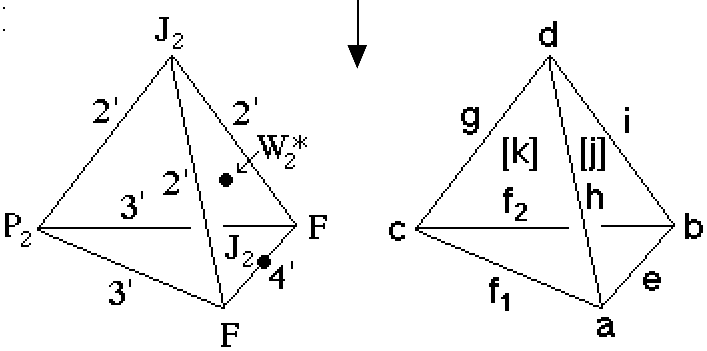
<u>Underlying Space S^3</u>



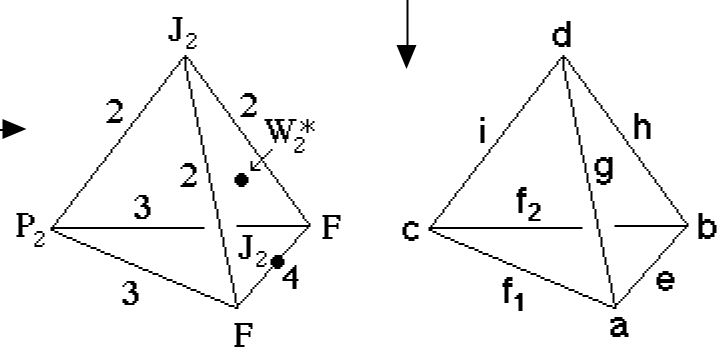
221 Pm$\bar{3}$m



207 P432



225 Fm$\bar{3}$m



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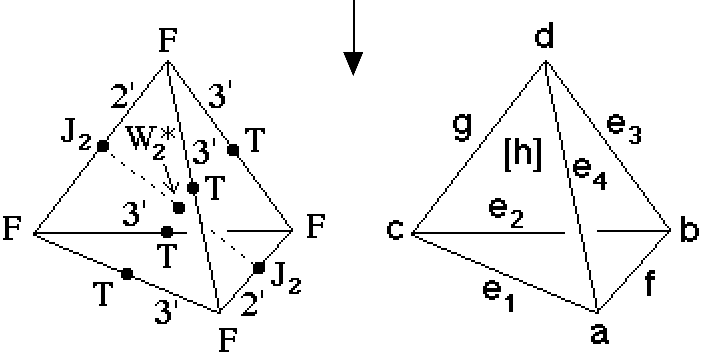
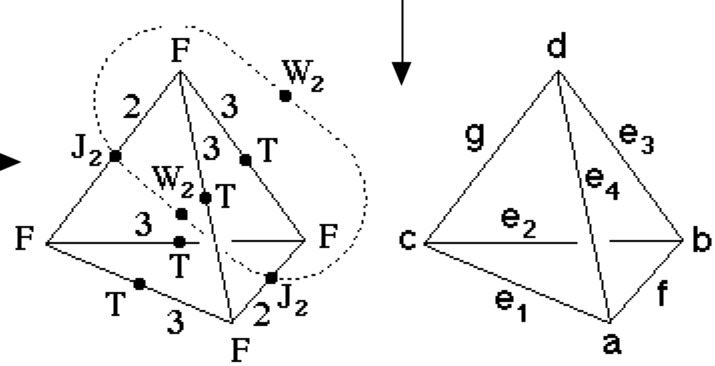


216 F$\bar{4}$3m

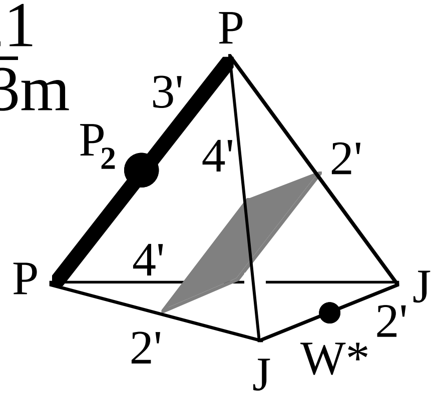


196 F23

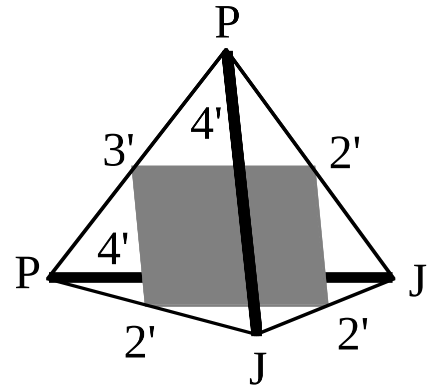
Normal Quadrilateral Heegaard Surfaces for the Three Nonorientable Tetrahedral Cubic Orbifolds

(Labels = Structure Type-Heegaard Surface-Critical Point Set)

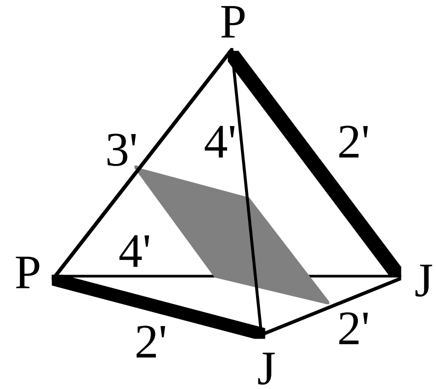
221
$Pm\bar{3}m$



CsCl
H4'2'4'2'm{1}
PP/P_2/W*/JJ

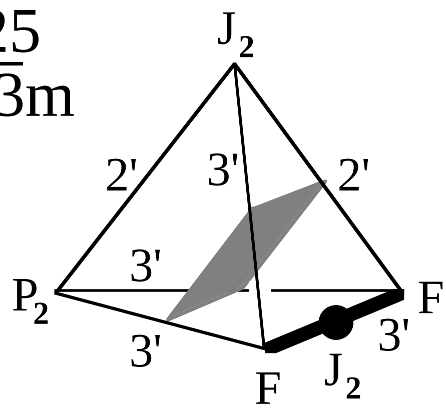


Simple Cubic
H3'2'2'm{2'}
P/J/J/P

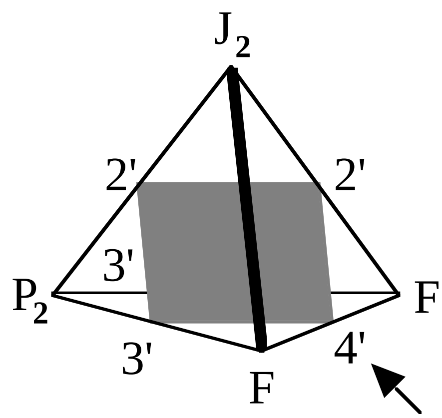


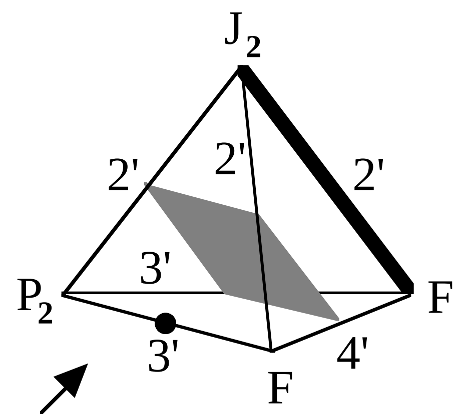
Invalid!!
H4'3'4'm{2'}
P/J/J/P

225
$Fm\bar{3}m$



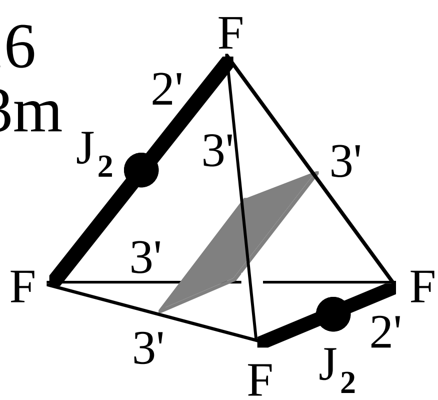
NaCl
H3'3'2'2'm{1'}
FF/J_2/J_2/P_2



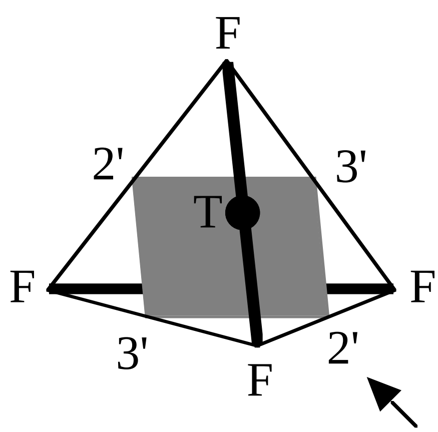


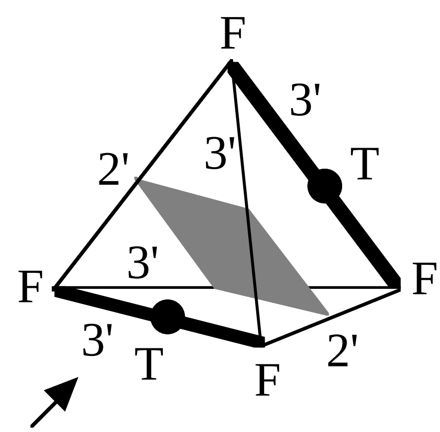
FCC
H4'3'2'2'm{1'}
F/J_2/3'/FP_2

216
$F\bar{4}3m$



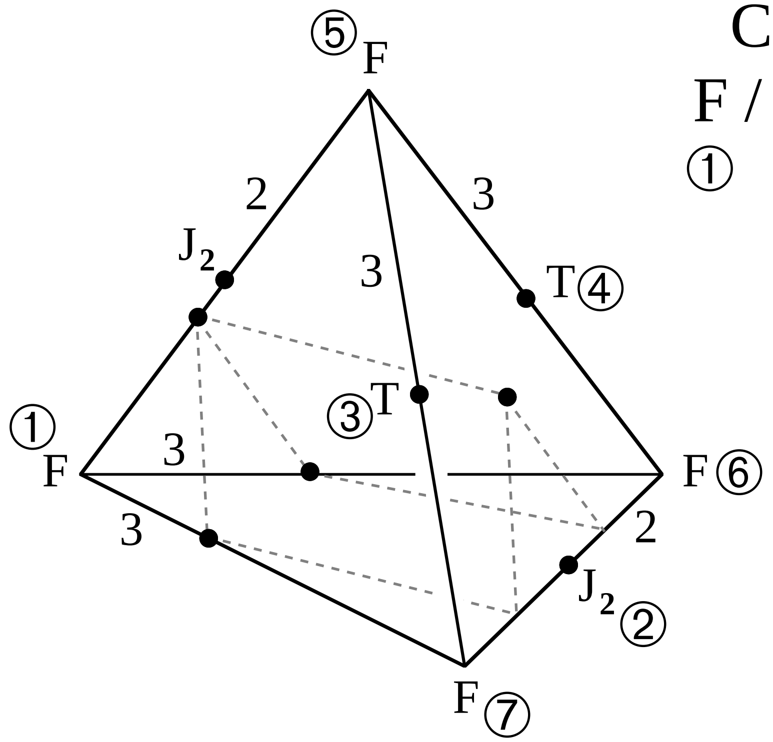
NaCl
H3'3'3'3'm{1}
FF/J_2/J_2/FF





ZnS
H3'2'3'2'm{1}
FF/T/T/FF

FCC Heegaard Splitting of the F23 3-Orbifold



Critical Points

F / J_2 / T T / F F F

① ② ③④ ⑤⑥⑦

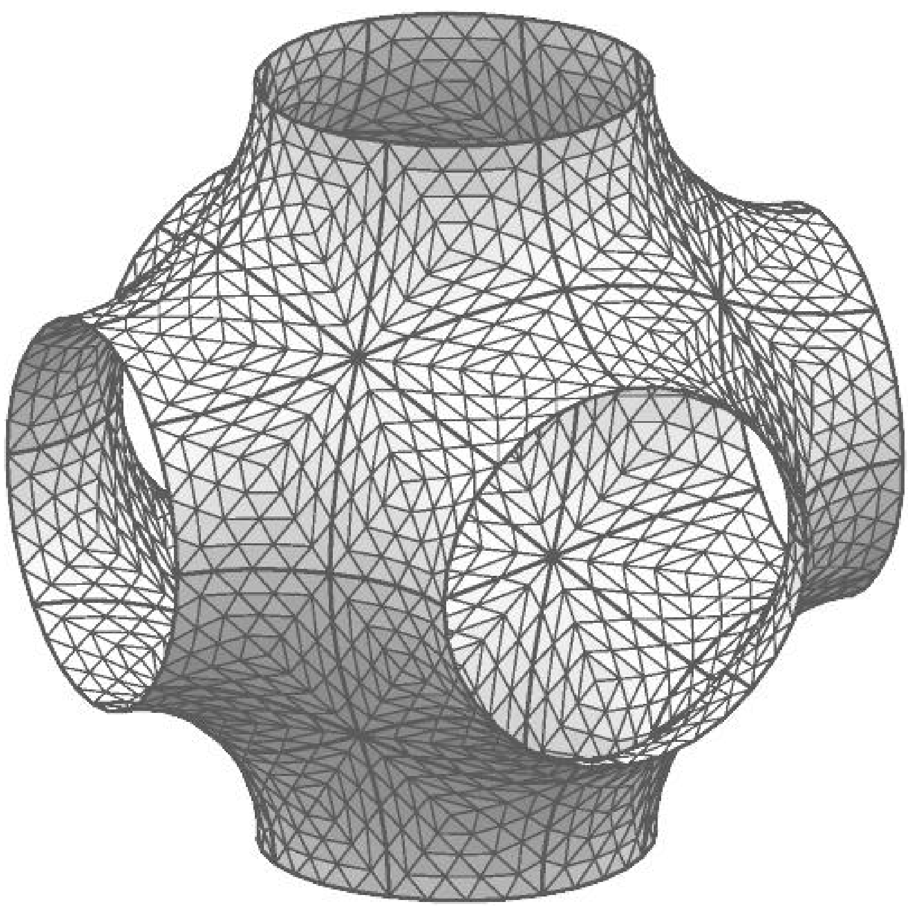
32<3>2<3>32 (-) handlebody
H33222{11} Heegaard surface
332<1>22 (+) handlebody

Note: A partitioning along ①,②,⑤ forms subtetrahedra ①,②,⑤,⑦ and ①,②,⑤,⑥, which can each undergo a quadrilateral normal surface splitting. When the pieces are properly recombined, the Heegaard splitting shown here is produced. Arbitrarily complex critical nets (crystal structures) on any crystallographic space group 3-orbifold can be split into tetrahedra for normal (or “almost normal”) surface analysis.

The Simple-Cubic Heegaard Surface Approximates Schwartz's P Surface (A Triply Periodic Minimal Surface)

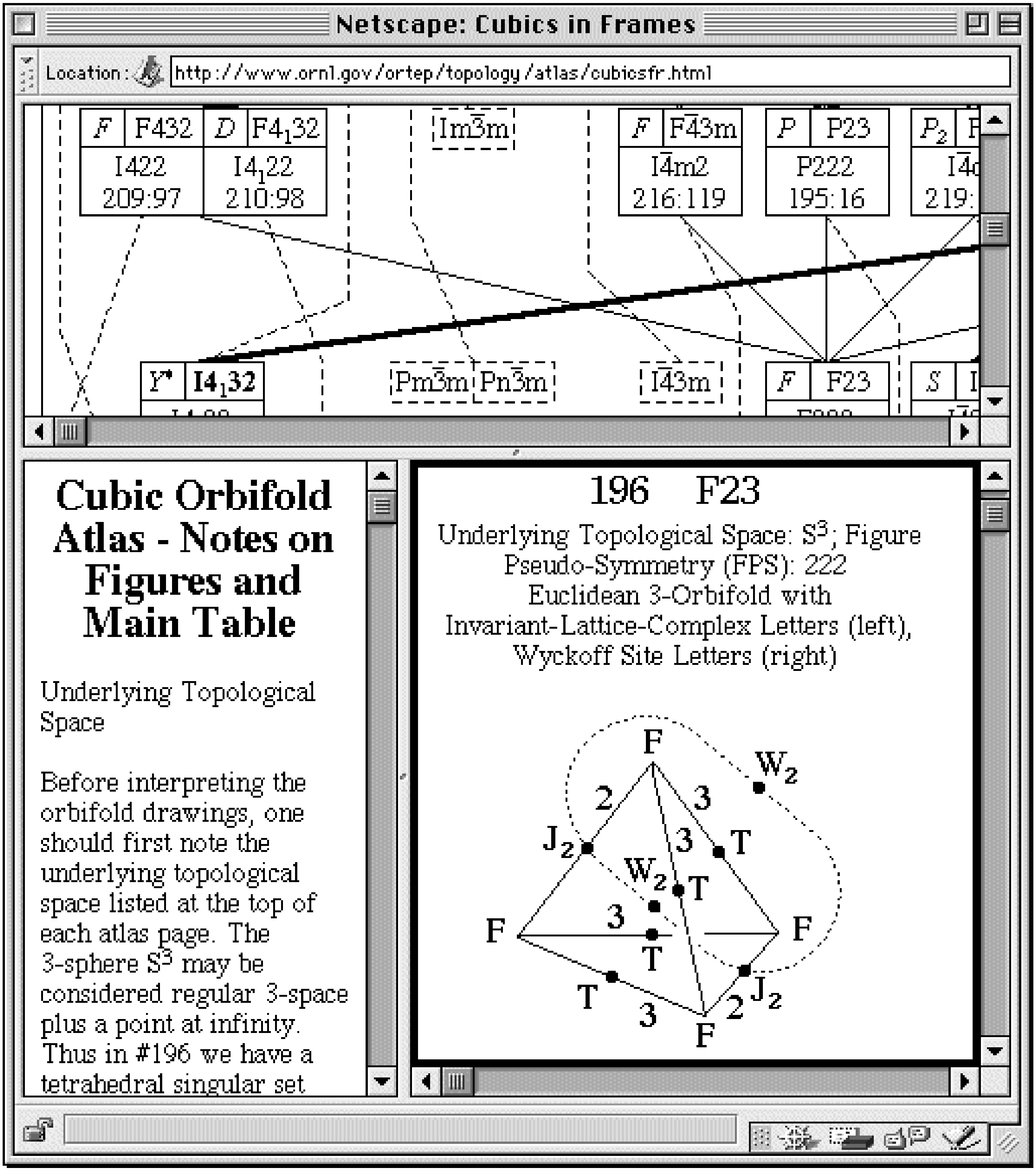
Unit cell drawing from Brakke's Surface Evolver program
Reference:http://www.susqu.edu/FacStaff/b/brakke/evolver/examples/periodic/periodic.html

Heavy lines are mirrors of $Pm\overline{3}m$.
Note the H3'2'2'2'm surface motif.



Frames Option for Viewing
Cubic Orbifold Atlas

http://www.ornl.gov/ortep/topology/atlas/cubcsfr.html



Online Cubic Euclidean 3-Orbifold Atlas

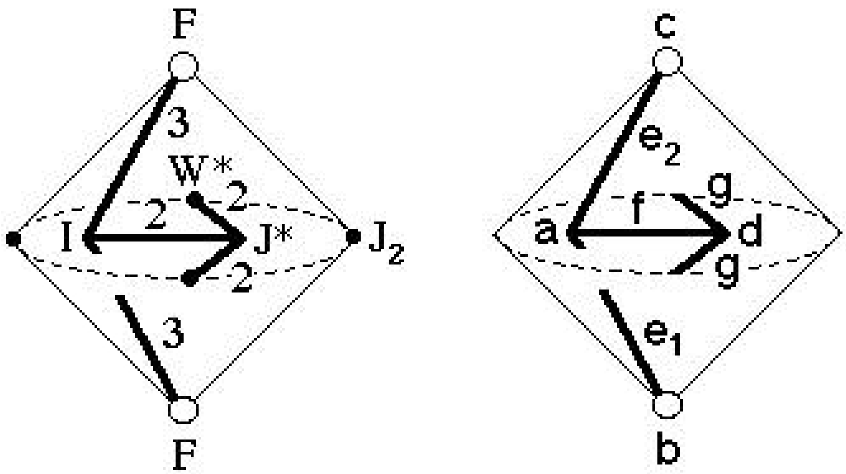
http://www.ornl.gov/ortep/topology.html

Two singular set 3-orbifold drawings on each orbifold with singular set and invariant lattice complex symbols. The following data provide analytical support for the drawings.

1. Underlying topological space.
2. Orbifold drawing pseudo-symmetry.
3. Wyckoff sets (of Wyckoff sites) based on group normalizer.
4. In-, uni-, di-, and trivariant lattice complexes and limiting lattice complexes grouped into characteristic (symmetry) and non-characteristic (pseudo-symmetry) singular sets.
5. Heegaard splitting examples.
6. Space group coordinates for invariant and limiting invariant lattice complex points.

Orbifold Atlas
201 Pn$\bar{3}$

Underlying Topological Space: RP^2 double suspension; Figure Pseudo-Symmetry (FPS): 2mm
Euclidean 3-Orbifold with Invariant-Lattice-Complex Letters (left), Wyckoff Site Letters (right)



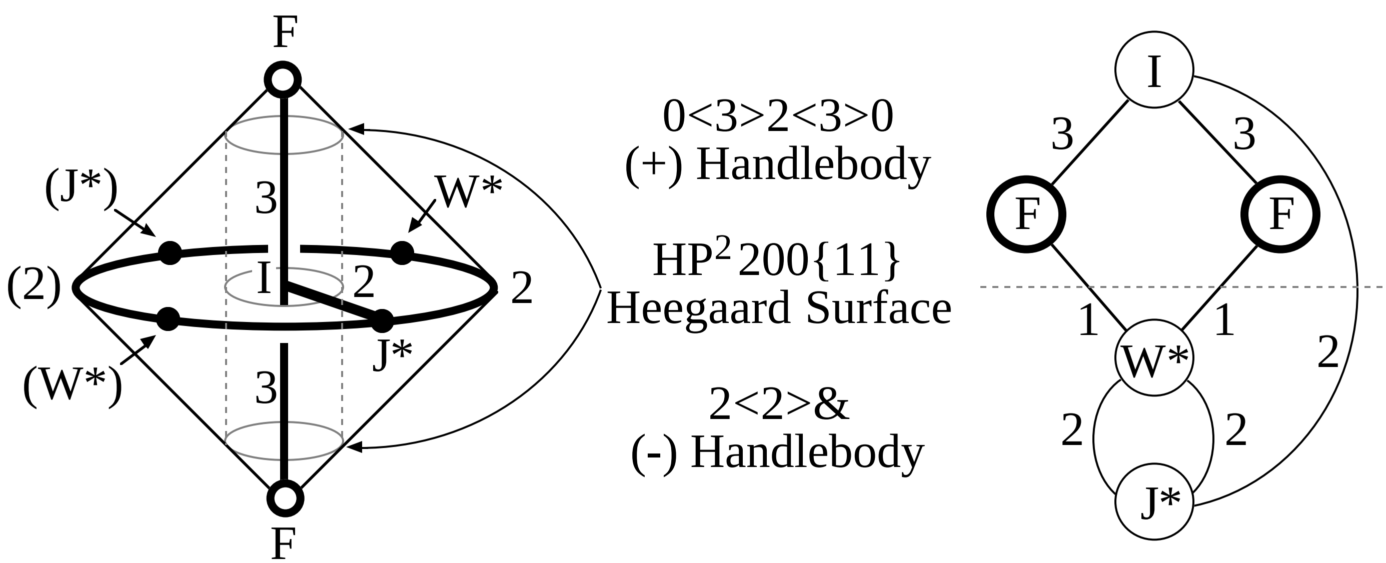
FPS	Mult	Lattice Comp	Group Graph	Wyckoff Set	2[4]Cover
	2-1	I	332	a	
	4-2	F	30	b, c	
	6-1	J*	222	d	
	8-2	I4[-]F2	32<3>0	(e1:b-a, e2:a-c)[1]	
	12-1	I6[-]J*2	33<2>22	(f:a-d)[2]	
	12-1	J*2[W*]&	2<2>&	(g:d-d)[3]	
	24		1	h:efg	
2	24-1	I12[J_2]J*4	2*=332<1>222	(h1:a-d)[4]	#222(h)
	24-1	F6[J_2]F6	2*=30<1>30	h2:b-c	[#202(e)]
	24-1	F6[-]W*2	2*=30<1>30	h3:b-g, h4:c-g	#224(i,j)
m	24-1		m*	(h5:fgh1)[5]	#204(g)
m	24-1		m*	(h6:eh2)[6]	#224(k)

Struct-Mult	Critical Points	Heegaard Surf	Wyckoff Cut
BCC -1	I/FF/W*/J*	HP^2 200{11}	f

Lattice Points: (1) 0,0,0 + (1/4,1/4,1/4) x2; (2) 1/4,1/4,1/4 + (0,1/2,1/2); (3) 1/4,3/4,3/4 + (-1/4,0,0) &; (4) 1/4,1/4,1/4 + (0,-1/4,-1/4) x2: (5) 1/4,y,z; (6) x,x,z

Heegaard Splitting of BCC Critical Net on Pn$\bar{3}$ 3-Orbifold

Topological Space: Double Suspension Real Projective Plane (RP^2)



Antipodal Cone Double Suspension [W* = (W*), J* = (J*), 2 = (2)]

Critical Net on Orbifold

Summary and Conclusions

Orbifold Atlas

- At http://www.ornl.gov/ortep/topology.html
- Scope- Cubic space groups (at present)
- Contents for each space group
  - Orbifold singular set topology drawings
  - Tabular data on
    - Characteristic singular set
      = Space group symmetry
    - Non-characteristic singular set
      = Space group pseudo symmetry
    - Wyckoff splitting examples
      $\rightarrow$ Possible basis set for all structures

Theory (or Understanding) Needs

- Heegaard transmutation methods
- Normal surface equations

Computer Automation Needs

- Orbifold data for remaining space groups
- Critical net derivation for known structures
- Heegaard transmutation mechanics
- Normal surface mechanics