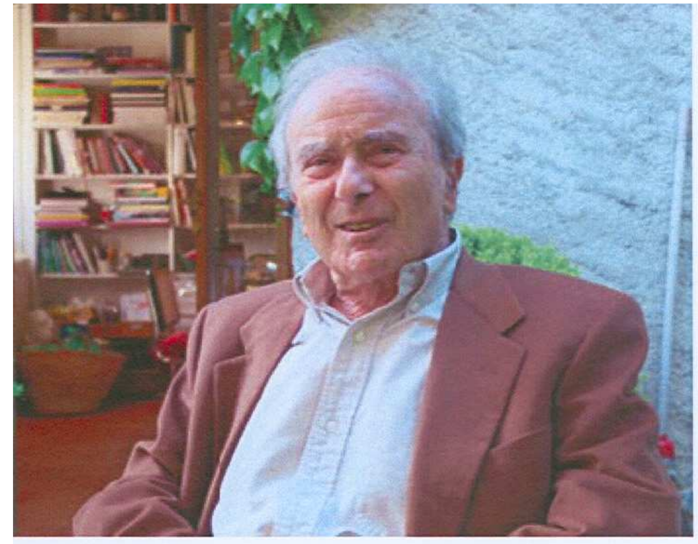
Experiencing Space Groups

1. Material research at Battelle, Geneve
2. Algebraic crystallography
3. Geometric crystallography
4. Arithmetic crystallography
5. Metric and dimensions
6. Molecular crystallography
7. The great family

   Higher-dimensional space groups
8. Documents and recollections



Edgar Ascher

80 years

XXI IUCr, Osaka, 30.08.08, In honour of Edgar Ascher A. Janner

Overview

Battelle Memorial Institute, Geneva
(Columbus, Ohio)

Aim : Research laboratory for industry (Non for profit)

Gordon Battelle, 1929

Groups : (1957)

- Physics : Philip Choquard
- Mathematics : Beno Eckmann, ETH

Projects : (1960)

Why Cobalt for magnetic materials Edgar Ascher

....

The Beginning

"Cobalt ions in non-metallic strucures"

1962-1963, E. Ascher & A. J., Battelle Report

Close-packed structures :

1611 J. Kepler, Seu de Nive Sexangula

....

1958 A.F. Wells, Crystal structures
Solid State Physics, vol.7, 425-503

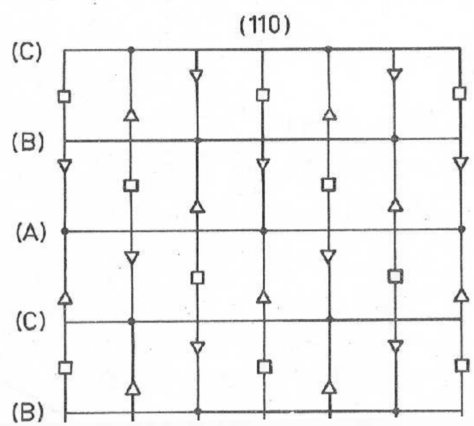
Structurebericht types, Structure types :

1931 P. Ewald & C. Hermann, Structurbericht,
Akademie Verlag, Leipzig

....

2007 P. Allmann & R. Hinex, The introduction of structure types into the Inorganic Crystal Structure Database ICSD, Acta Cryst, A63, 411

Structurberict type C1, CaF_2 Structure



$(1\ 0\ 1\ 1)_c$ Ca F F

c □ △ ▽ c △ ▽

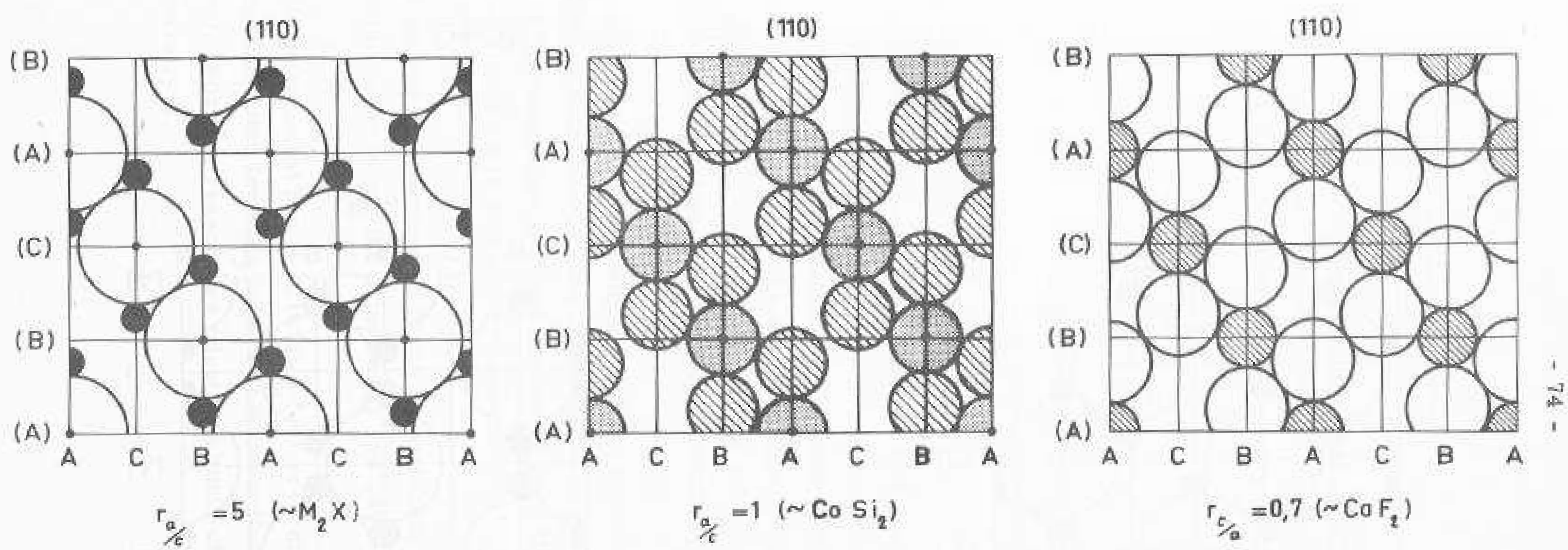


Fig. B10: Limiting cases of compact anionic structures (cubic close-packing and simple cubic packing) and intermediate one in crystals of the SB type C1, CaF_2 structure.

Space Group G

Abstract G **:** $\Lambda \subset G$

Λ $\begin{cases} \text{free abelian} \\ \text{maximal abelian} \\ \text{normal subgroup} \end{cases}$

$G/\Lambda \simeq K$ finite

Euclidean G **:**

$G \subset E^n$ — E^n Euclidean group of $\mathbb{R}^n$

$\Lambda = G \cap T^n$ — $T^n \subset E^n$ group of translations

Λ group of lattice translations which generates $V(n, \mathbb{R})$

$G/\Lambda \simeq K \subset O(n, \mathbb{R})$ — K point group of G

$O(n, \mathbb{R})$ Orthogonal group

Group Extension

Short exact sequence :

$$0 \longrightarrow \Lambda \xrightarrow{\kappa} G \xrightarrow{\sigma} K \longrightarrow 1 \qquad \text{Exact : } Im(\kappa) = Ker(\sigma)$$

Factor set $m: \ K \times K \longrightarrow \Lambda$

$$\boxed{(a,\alpha)(b,\beta) = (a + \varphi(\alpha)b + m(\alpha,\beta), \alpha\beta)}$$

$\varphi : K \longrightarrow Aut(\Lambda)$ monomorphism

$(a,\alpha),(b,\beta) \in G \quad a, b \in \Lambda, \quad \alpha,\beta \in K$

Equivalent factor set : $(a,\alpha) \rightarrow (a + c(\alpha), \alpha)$

$$\boxed{m'(\alpha,\beta) = c(\alpha) + \varphi(\alpha)c(\beta) + c(\alpha\beta) + m(\alpha,\beta)}$$

Extension group $Ext(\Lambda, K, \varphi)$ **:**

Equivalence classes of extensions G of abelian Λ by finite K and $\varphi(K) \subset Aut(\Lambda)$

Cohomology

Cochains : $f^n \in C^n_\varphi(B,A)$

$$f^n : B \times B \times ... \times B \longrightarrow A \qquad \varphi(B) \subset Aut(A)$$

Coboundary operators : δ_n

$$A \xrightarrow{\delta_0} C^1_\varphi(B,A) \xrightarrow{\delta_1} C^2_\varphi(B,A) \xrightarrow{\delta_2} ...., \qquad \delta_n\delta_{n-1} = 0$$

Coboundaries : $Im\ \delta_{n-1} = B^n_\varphi(B,A)$

Cocycles : $Ker\ \delta_n = Z^n_\varphi(B,A)$

Cohomology groups : $H^n_\varphi(A,B) = Z^n_\varphi B, A)/B^n_\varphi(B,A)$

Factor set : m: 2-cocycle $\quad m' - m$: 2-coboundary

$$\boxed{H^2_\varphi(K,\Lambda) \simeq Ext(\Lambda, K, \varphi)}$$

Non-Primitive Translations

Commutative diagram :

$$\begin{array}{ccccccccc} 0 \to & \Lambda \to & G \to & K \to 1 \\ & \downarrow & \downarrow & \downarrow \\ 0 \to & T^n \to & E^n \to & O^n \to 1 \end{array}$$

Euclidean motion : $(a, \alpha) = \{\alpha | u(\alpha)\} \in G$ Seitz notation

$$\{\alpha | u(\alpha)\}\, x = \varphi(\alpha) x + u(\alpha), \quad x \in V^n$$

Change of coset representative : $u'(\alpha) = a + u(\alpha), \quad a \in \Lambda$

Non-primitive translation : $u(\alpha)$

$$u(\alpha\beta) = \varphi(\alpha)\, u(\beta) + u(\alpha) \quad u \in Z^1_\varphi(K, T^n/\Lambda)$$ 1-cocycle

Change of origin : $u'(\alpha) = u(\alpha) + f - \varphi(\alpha) f = u(\alpha) + \delta f$

$$\delta f \in B^1_\varphi(K, T^n/\Lambda)$$ 1-coboundary

$$\boxed{[u] \in H^1_\varphi(K, T^n/\Lambda)}$$ $[u]$ vector set

Space Group Cohomology

Exact sequences :

$$\begin{array}{ccccccc} H^1_\varphi(K,T^n) & \rightarrow & H^1_\varphi(K,T^n/\Lambda) & \rightarrow & H^2_\varphi(K,\Lambda) & \rightarrow & H^2_\varphi(K,T^n) \\ \| & & \downarrow & & \downarrow & & \| \\ 0 & \rightarrow & H^1_\varphi(K,T^n/\Lambda) & \rightarrow & H^2_\varphi(K,\Lambda) & \rightarrow & 0 \end{array}$$

$$\boxed{H^1_\varphi(K,T^n/\Lambda) \simeq H^2_\varphi(K,\Lambda)}$$

$\nearrow$ Non-primitive translations: vector set u

$\nwarrow$ Group extension: factor set m

H1 iso H2

Reals, (Rationals), Integers

Choice of a basis : $b = \{b_1, \ldots, b_n\}$, basis of the lattice Λ

$$t = \sum_i^n r_i b_i = [r_1, \ldots, r_n] \in V(n, \mathbb{R}), \quad r_i \in \mathbb{R}$$
$$a = \sum_i^n z_i b_i = [z_1, \ldots, z_n] \in \Lambda, \quad z_i \in \mathbb{Z}$$

$$T^n \simeq \mathbb{R}^n, \qquad \Lambda \simeq \mathbb{Z}^n, \qquad T^n/\Lambda \simeq \mathbb{R}^n/\mathbb{Z}^n$$
$$O^n \simeq O(n, \mathbb{R}), \qquad K \simeq \varphi(K) \subset O(n, \mathbb{R})$$

Arithmetic : $Gl(n, \mathbb{Z})$ arithmetic group

$$Aut(\Lambda) \simeq Gl(n, \mathbb{Z}), \qquad \varphi(K) \subset Gl(n, \mathbb{Z})$$

$\varphi(\alpha) = A(b), \;\; \alpha \in K$ $\quad$ $A(b)$ integral invertible matrix

Metric : $g_{ik}(b) = b_i \cdot b_k$ Gram matrix (metric tensor)

$$A(b) g(b) \tilde{A}(b) = g(b) \qquad A(b) \in \varphi(K) \subset O(n, \mathbb{R})$$

Metric - Arithmetic Interplay

Crystal Class : $K \overset{geom}{\sim} K'$ geometric equivalent point group

$$K \overset{geom}{\sim} K' \Longleftrightarrow K' = RKR^{-1}, \quad R \in O^n$$

Arithmetic Class : $K \overset{arith}{\sim} K'$ arithmetic equivalent point group

$$\varphi(K) \overset{arith}{\sim} \varphi'(K') \Longleftrightarrow \varphi'(K') = B\varphi(K)B^{-1}. \quad B \in Gl(n, \mathbb{Z})$$

Lattice Holohedry : $H(\Lambda)$ point group symmetry of Λ

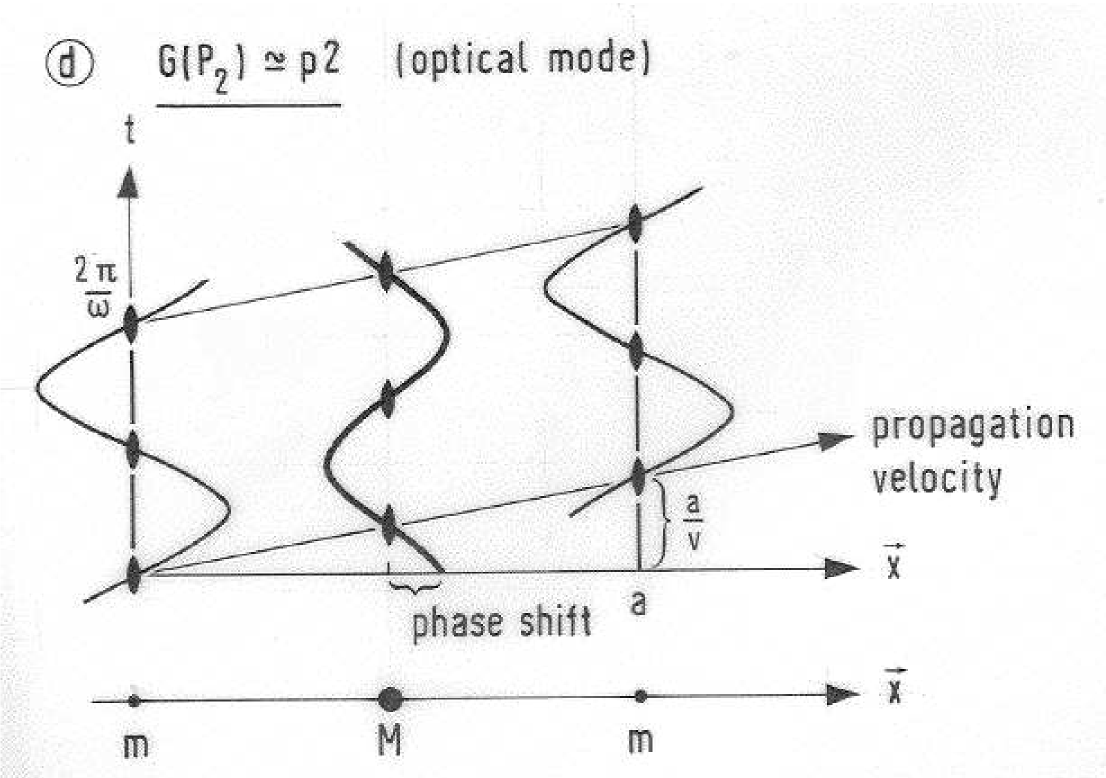
$$H(\Lambda) = \{R\Lambda = \Lambda \mid \forall R \in O^n\}$$

Bravais class : $\Lambda' \overset{Bravais}{\sim} \Lambda$

$$\boxed{H'(\Lambda') \overset{arith}{\sim} H(\Lambda) \Longleftrightarrow \Lambda' \overset{Bravais}{\sim} \Lambda}$$

Space-Time Symmetry

Crystal Vibrational Mode



Laue diffraction

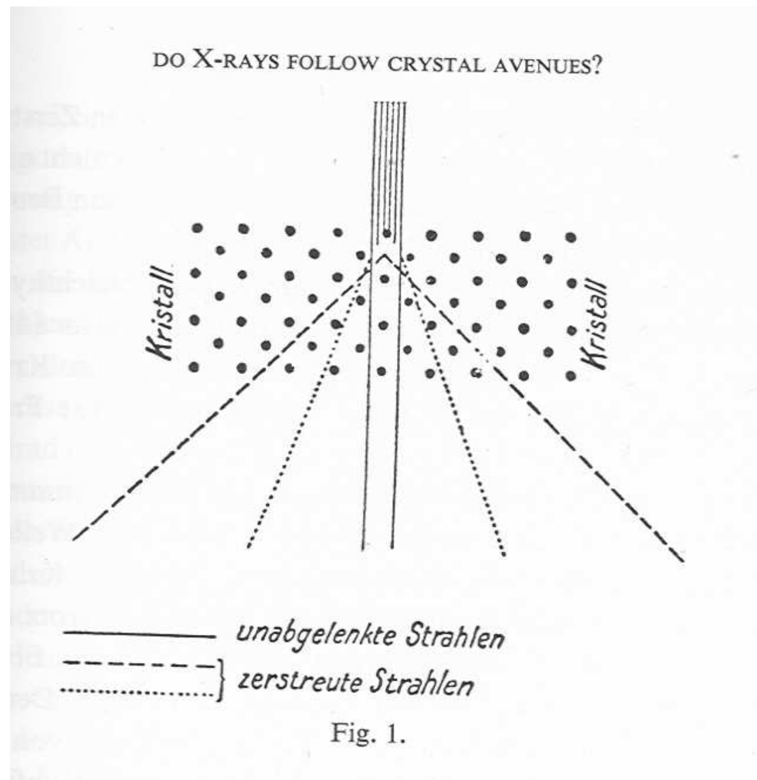


Fig. 1.

Incident ray + crystal
Diffracted rays + crystal

} same space-time symmetry

Rank and Dimension

Z-module basis b **:** rank n, dimension d

$$a = z_1 b_1 + \ldots + z_n b_n, \quad b \text{ linear independent on } \mathbb{Z}$$
$$t = r_1 b_1 + \ldots + r_n b_n, \quad b \text{ generates } V^d \text{ on } \mathbb{R}$$

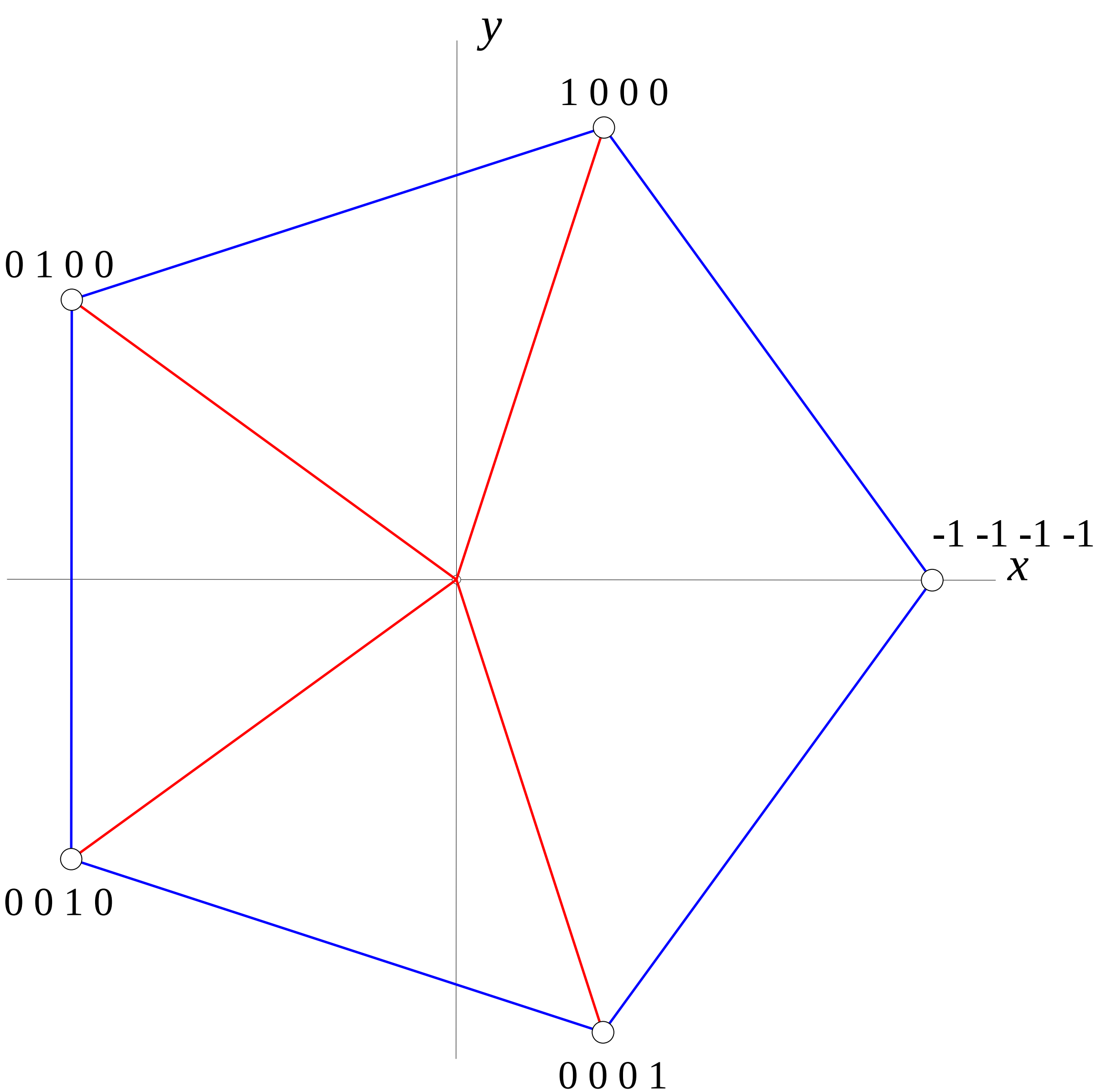
Z-module M **:** rank n, dimension d,

$$M = \{a = z_1 b_1 + \ldots + z_n b_n \mid \forall z_i \in \mathbb{Z}\}$$

Space group :	rank = dimension,	lattice $M = \Lambda$
Superspace group :	rank > dimension,	Z-module M

Rank

Pentagonal Symmetry



Pentagonal $\mathbb{Z}$-module

Basis vectors:

$$b_k = a(\cos k\phi, \sin k\phi)$$
$$\phi = \frac{2\pi}{5}, \quad k = 1, 2, 3, 4$$

Euler φ-function: $\varphi(5) = 4$

Rank 4, Dimension 2

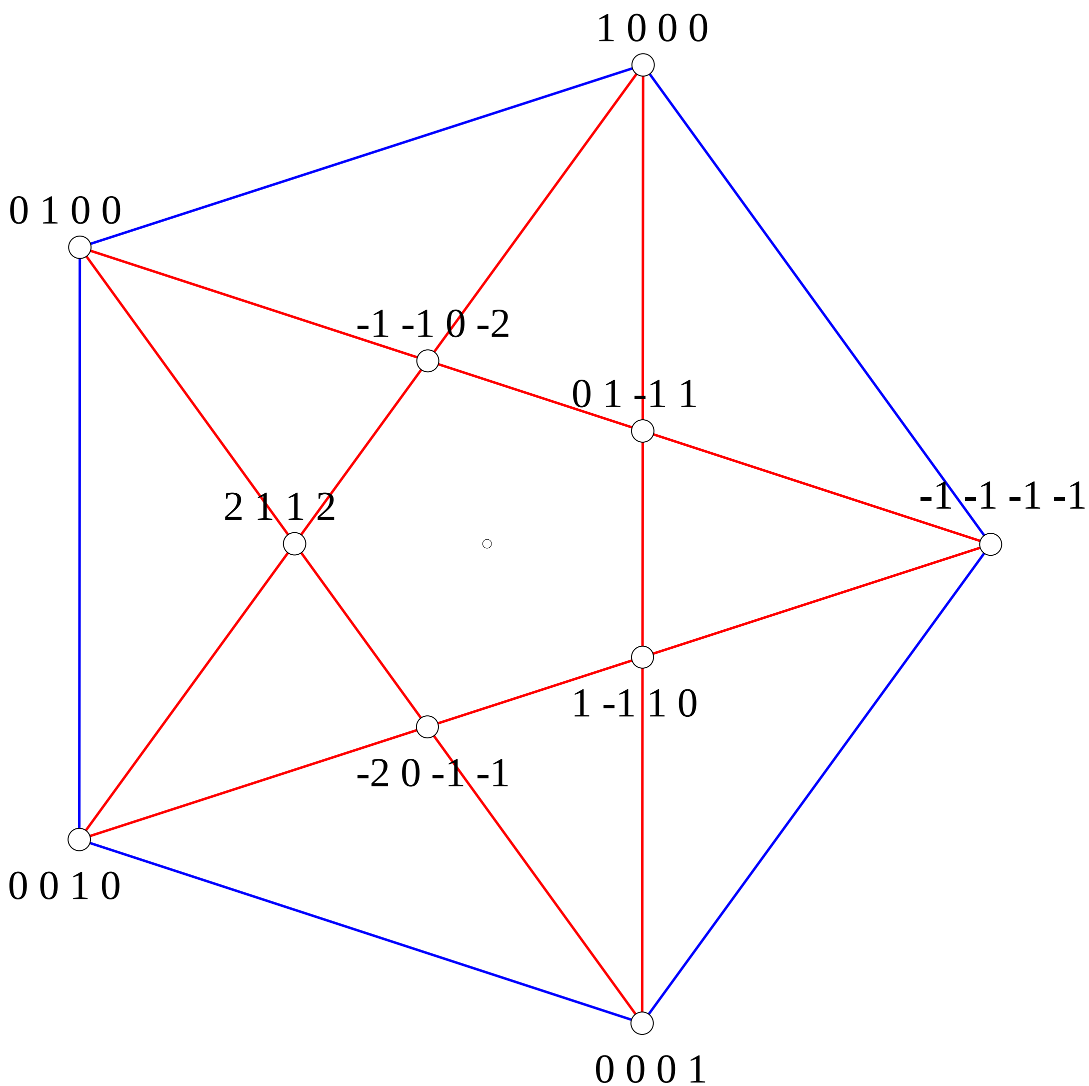
Positions:

$$P = (n_1, n_2, n_3, n_4)$$
$$= \sum_{i=1}^{4} n_i b_i$$

Indices: n_1, n_2, n_3, n_4

(integers)

Indexed Pentagram



Pentagrammal Scaling

Star Pentagon:

Schäfli Symbol {5/2}

Scaling matrix: (planar scaling)

$$\begin{pmatrix} \bar{2} & 1 & 0 & \bar{1} \\ 0 & \bar{1} & 1 & \bar{1} \\ \bar{1} & 1 & \bar{1} & 0 \\ \bar{1} & 0 & 1 & \bar{2} \end{pmatrix}$$

Scaling factor:

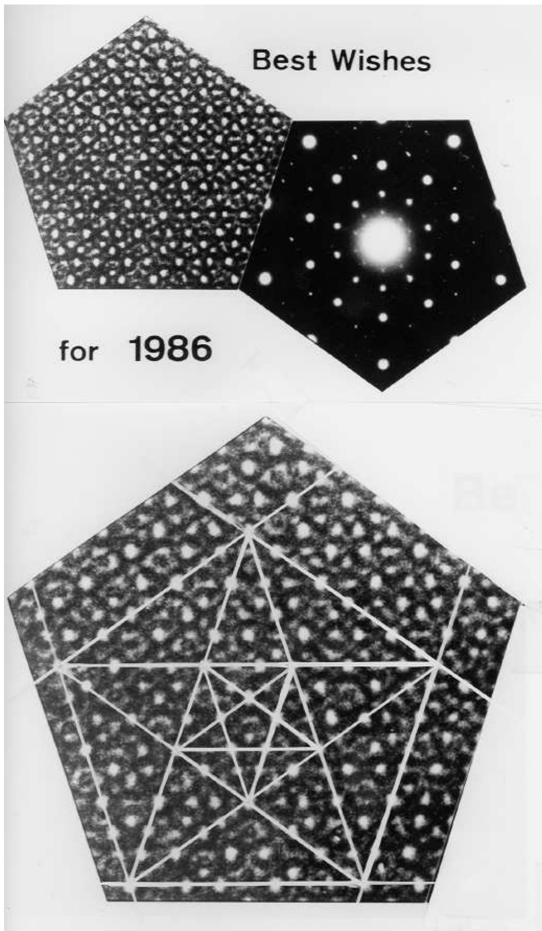
$$-1/\tau^2 = -0.3820...$$

$$(\tau = \frac{1+\sqrt{5}}{2} = 1.618...)$$

Pentagram

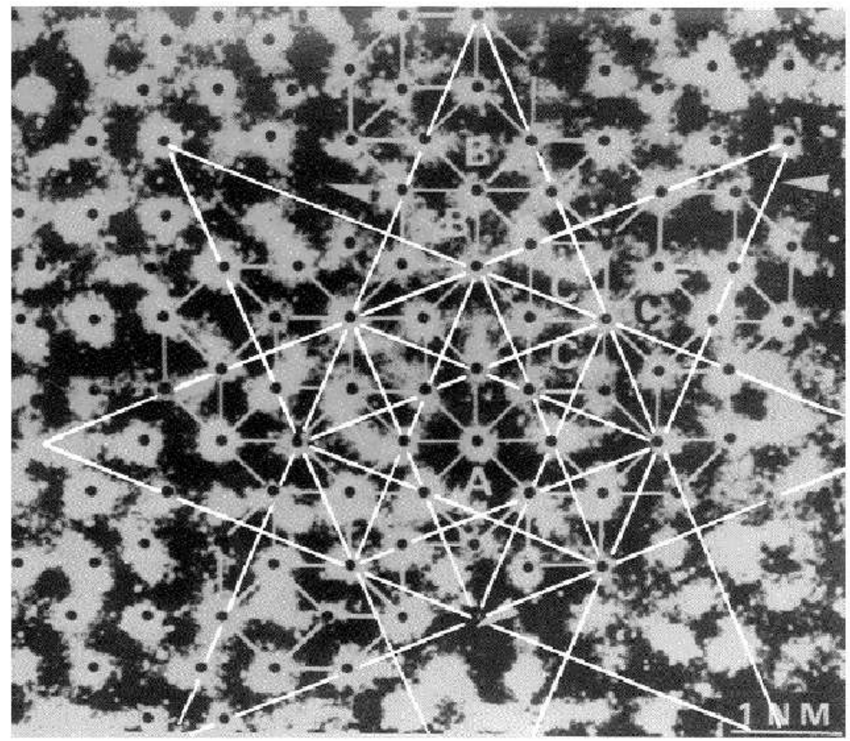
Pentagrammal Scaling Symmetry

Icosahedral Quasicrystal



First Decagonal Phase

(Kuo, XIV IUCr Conf., Perth, 1987)



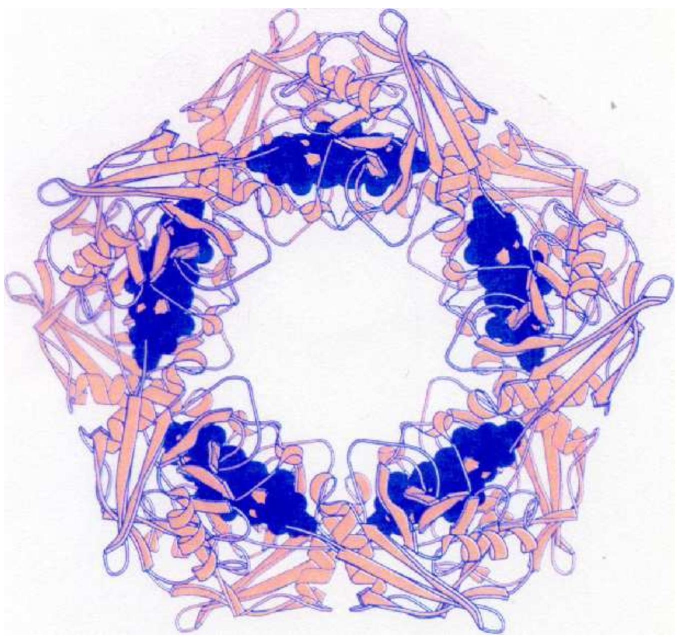
Superspace groups with infinite Point group ?

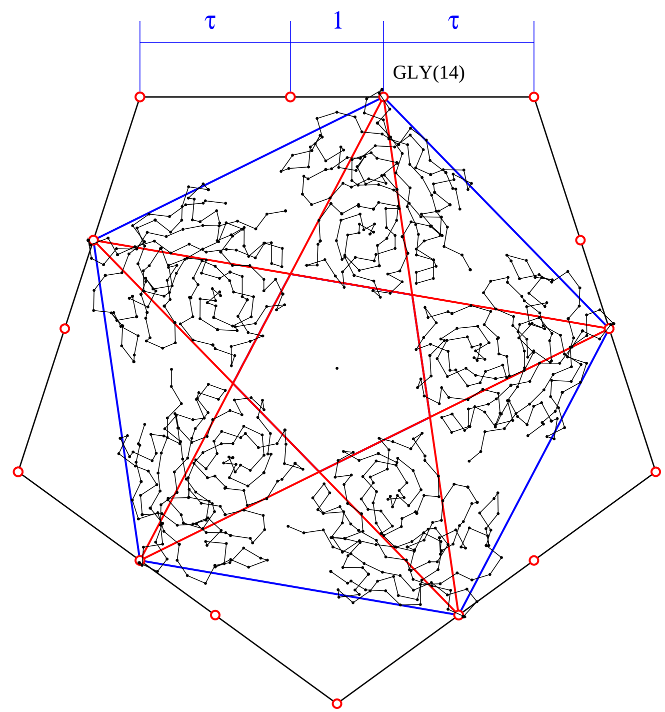
Classification ?

Pentagrammal Structural Relation

Cyclophylin - Cyclosporin Decamer

Cyclophylin Pentamer





Ke et al., Curr. Biology Struct., 2 (1994) 33

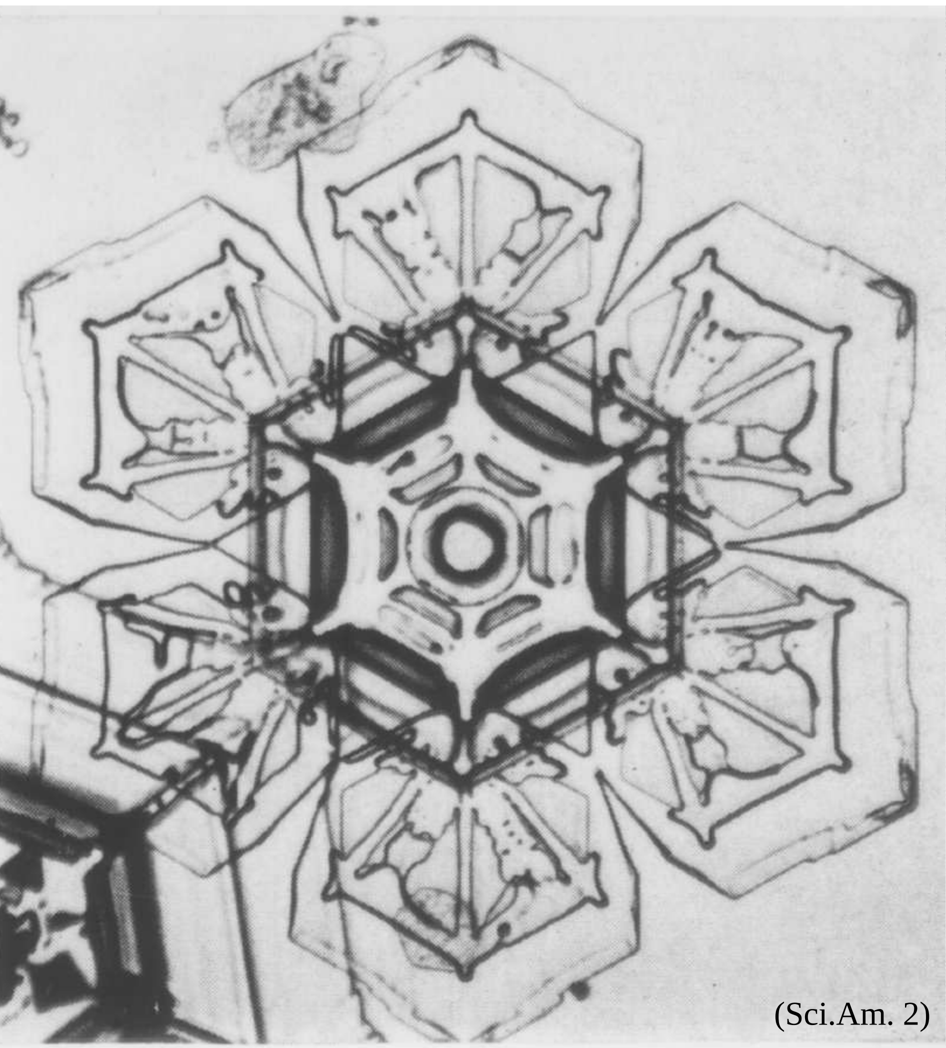
Ke and Mayrose (PDB 2rma)

Scaling cannot be a molecular symmetry !

Cyclophilin A

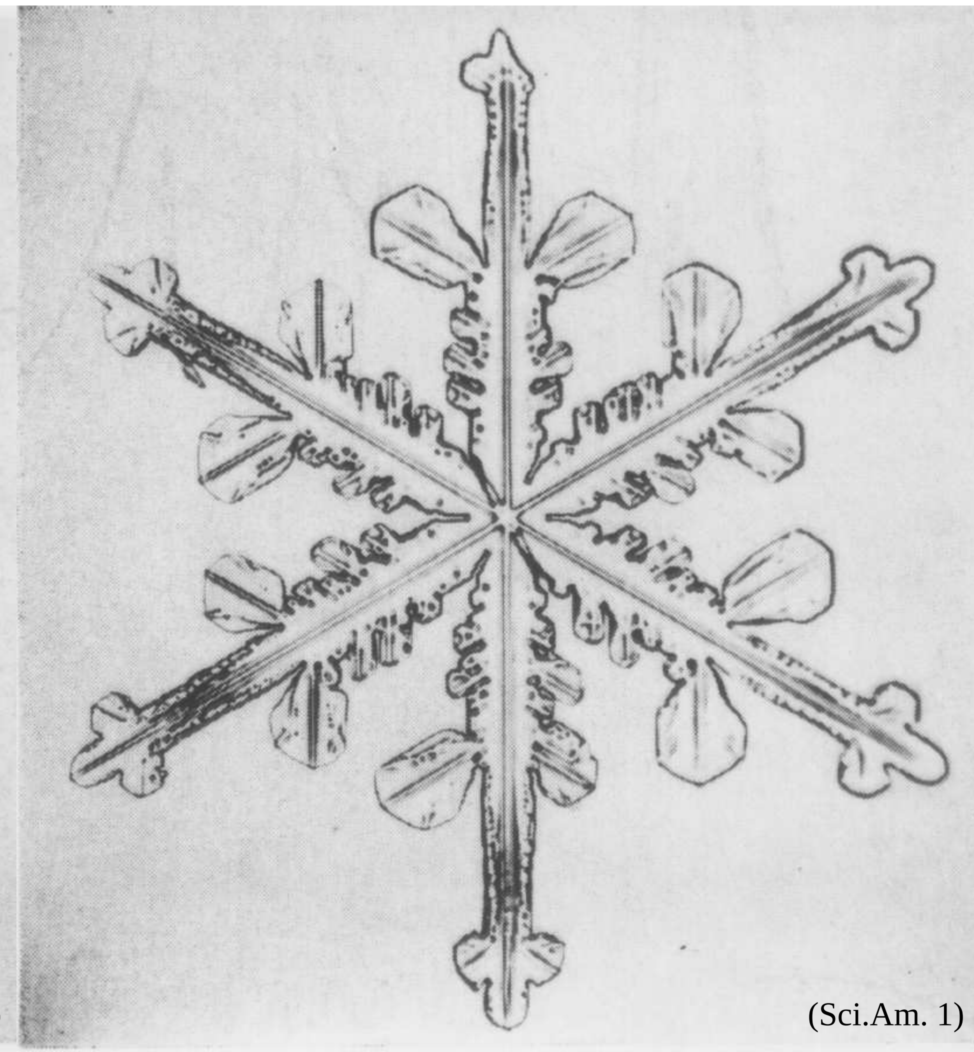
Hexagrammal Scaling in Snow Crystals

Facet-like snow flake



(Sci.Am. 2)

Dendritic-like snow flake

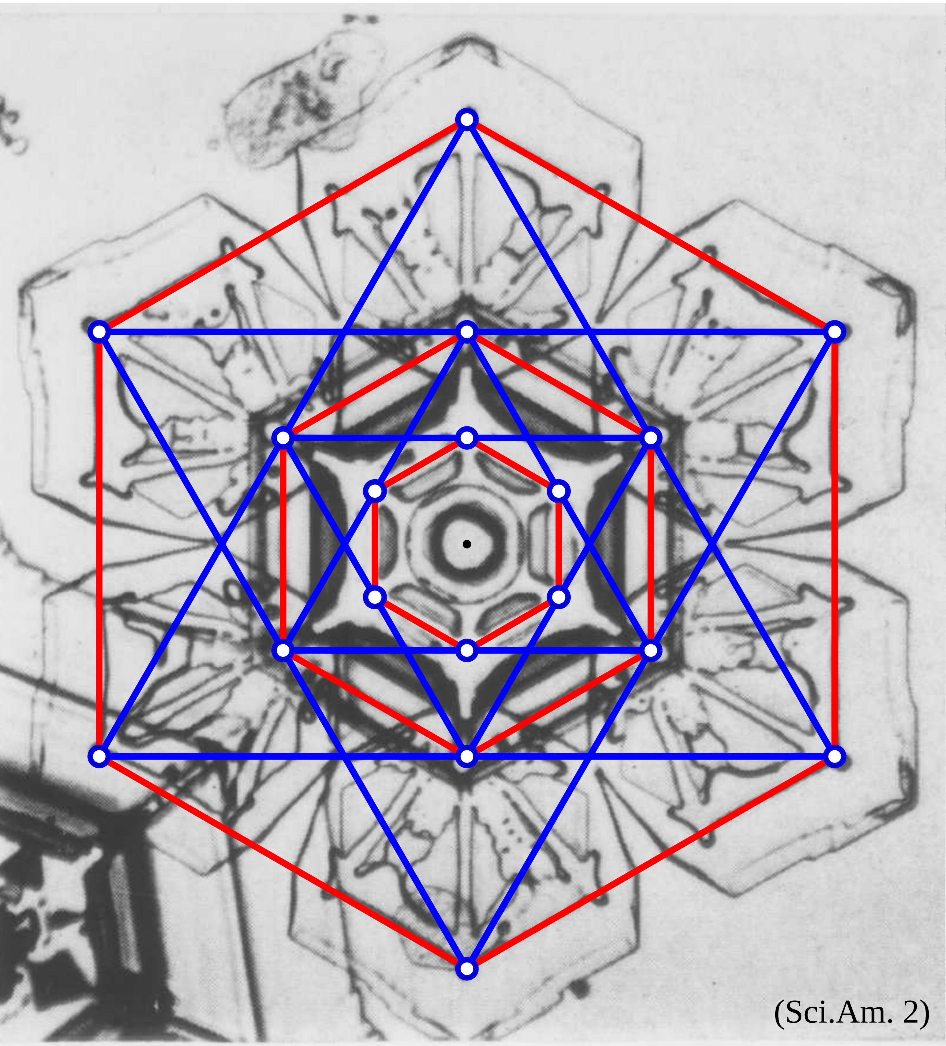


(Sci.Am. 1)

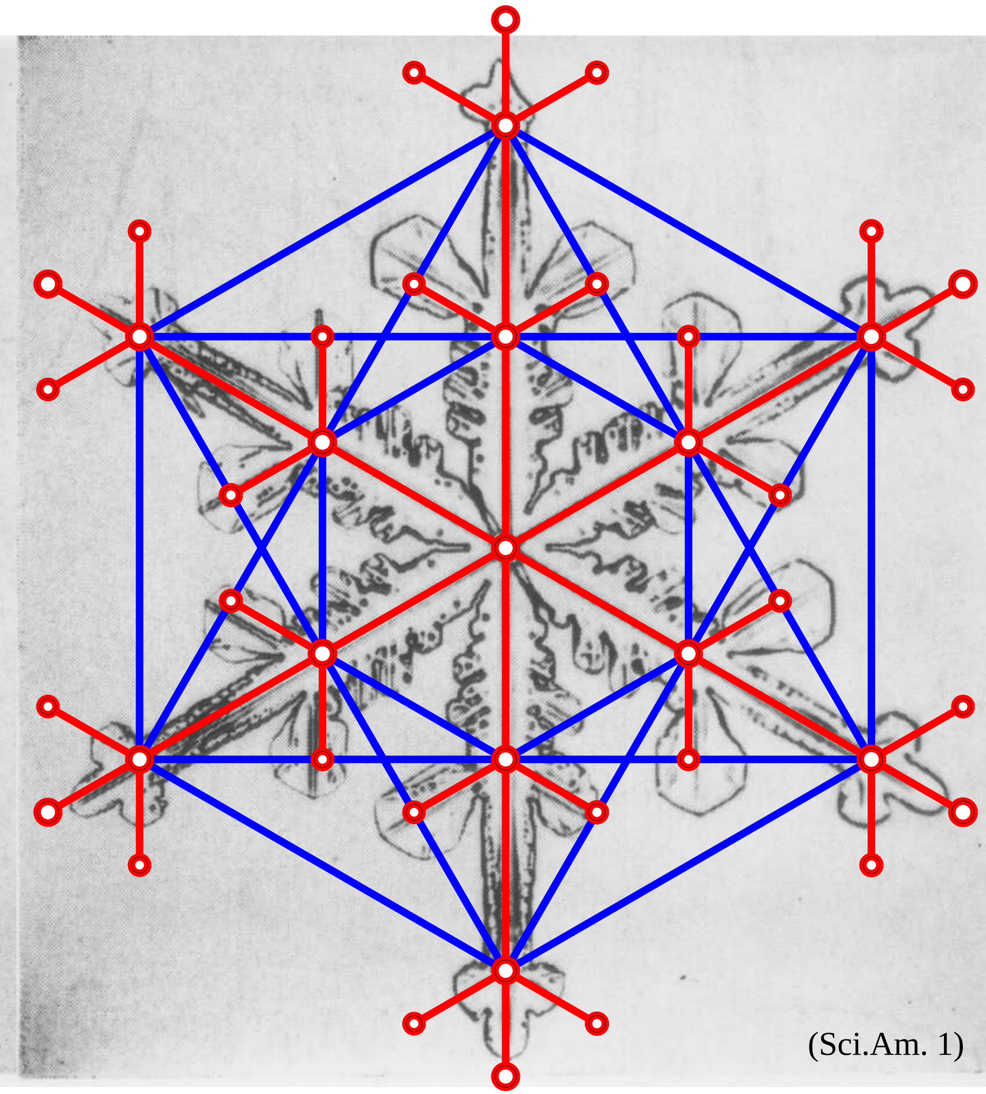
Sa1+Sa2[SAb]

Scientific American (1961)

Hexagrammal Scaling in Snow Crystals



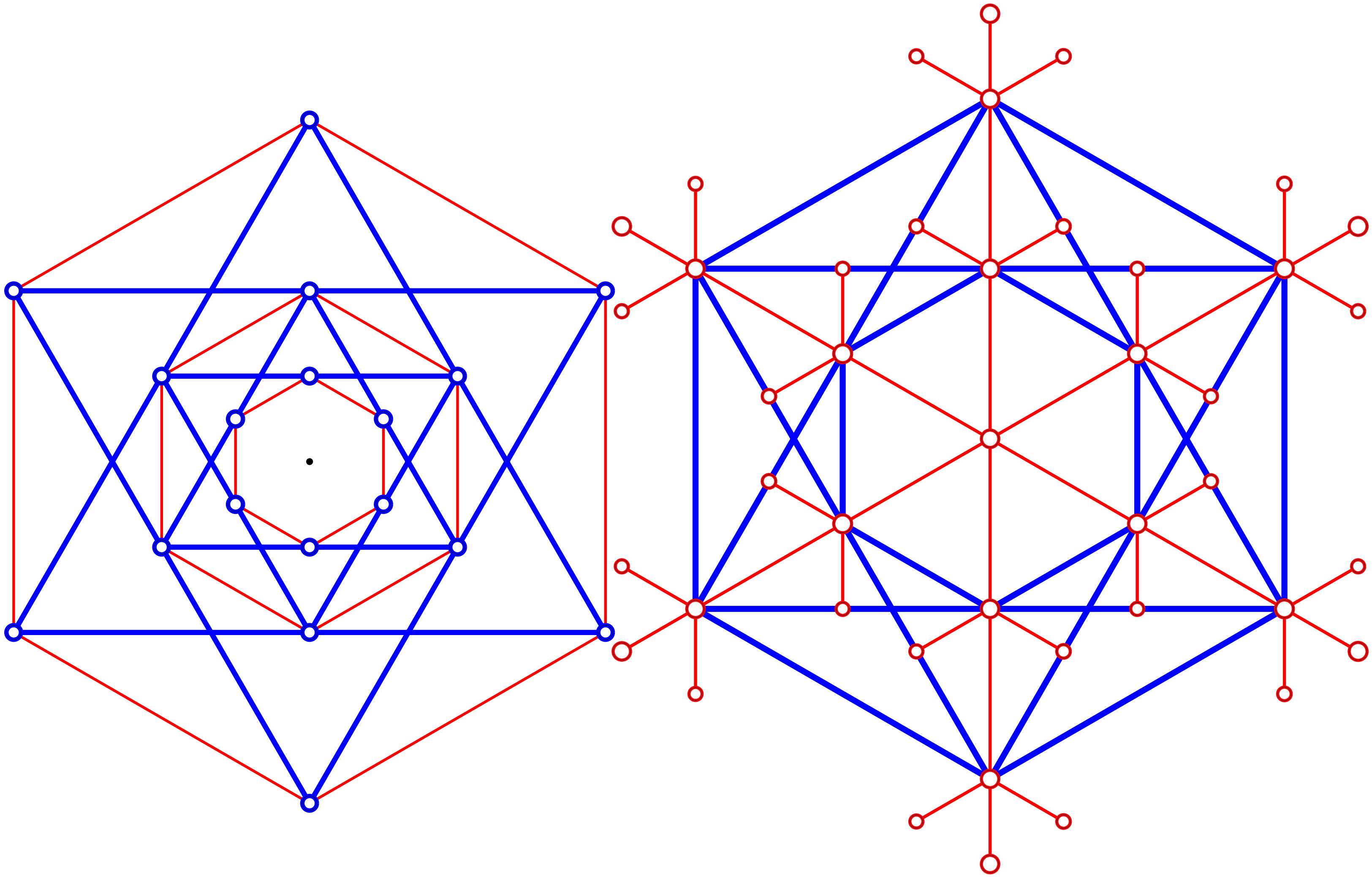
(Sci.Am. 2)



(Sci.Am. 1)

Sa1+Sa2[SAb]

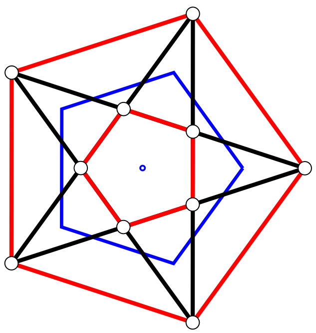
Hexagrammal Scaling in Snow Crystals



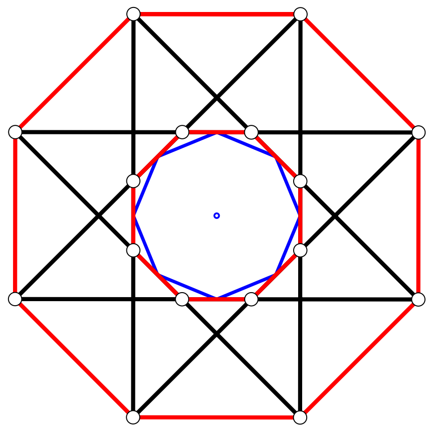
Sa1+Sa2[SAb]

Polygrammal Symmetry from Higher-Dimensional Point Groups

Dimension n, Point group K, Order $|K|$, Generating point P



(a)



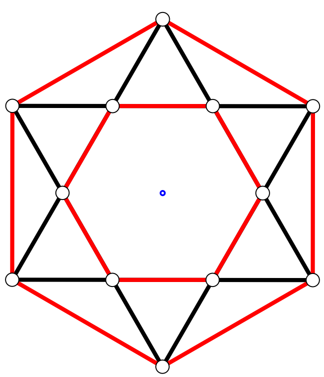
(b)

(a) Pentagram {5/2}

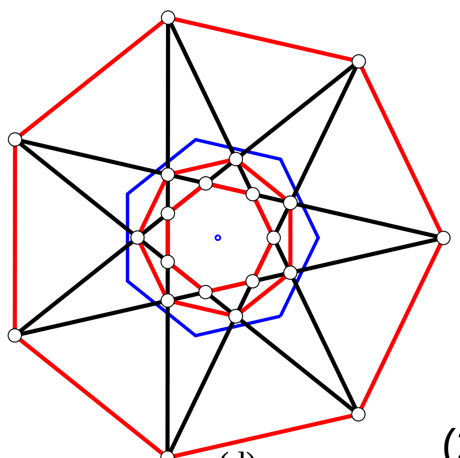
$n = 4$, $K \simeq 20.5$, $|K| = 20$, $P = [1100]$

(b) Octagram {8/3}

$n = 4$, $K \simeq 16.13$, $|K| = 16$, $P = [1100]$



(c)



(d)

(c) Hexagram {6/3}

$n = 3$, $K \simeq m\bar{3}m$, $|K| = 48$, $P = [1\bar{1}0]$

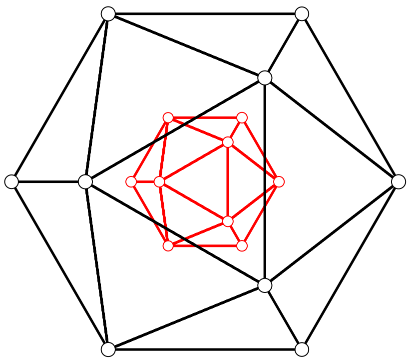
(d) Heptagrams {7/2}, {7/3}

$n = 6$, $K \simeq \ldots$, $|K| = 21$, $P = [111000]$

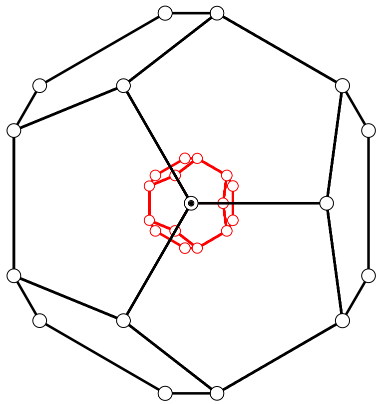
(20.5 and 16.13: BBNWZ, Crystallographic groups in four-dimensional space)

Polyhedral Cluster Symmetry

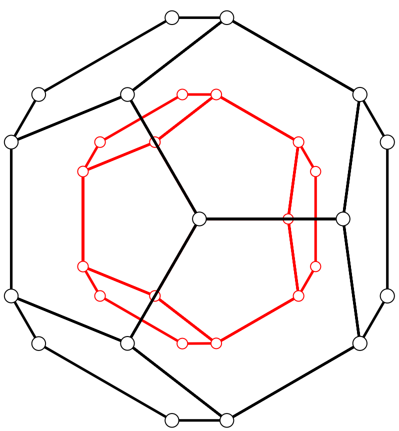
6 Dim. Point group $K = P2354$, Order $|K| = 240$, C_4 extension of 235



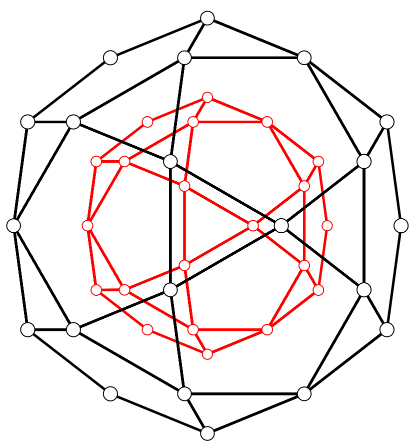
[1 1 1 1 1 1]
(a)



[1 1 1 0 0 0]
(b)



[1 1 1 1 1 -1]
(c)



[1 1 0 0 0 0]
(d)

235 Icosahedral group

(a) τ^2-scaled Icosahedra

(b) τ^3-scaled Dodecahedra

(c) τ-scaled Dodecahedra

(d) τ-scaled Icosidodecahedra

Higher-Dimensional Crystallography

Four-dimensional Point and Space groups

- Brown, Bülow, Neubüser, Wondratschek and Zassenhaus
  Crystallographic groups in four-dimensional space
  1978, Wiley, New York

Computer Algebra Programs

GAP

Groups, Algorithms and Programming

MAGMA

W. Bosma and J. Cannon, Sidney

CARAT

J. Opgenorth, W. Plesken and T. Schulz, Achen

1961 Battelle Memorial Institute Geneva, Carouge

Un système de translations non primitives pour une extension

$$0 \to Z^n \to G \to K \to 1$$

et un système de K à Z^n

$$(\varphi, m)$$

est un élément de

$$H^1_\varphi(K, R^n/Z^n),$$

Pour Z^n, K et φ données l'ensemble des extensions non-équivalents constitue

$$H^2_\varphi(K, Z^n) \quad ,$$

l'ensemble des systèmes des translations non primitives forme

$$H^1_\varphi(K, R^n/Z^n),$$

et ces deux groupes sont isomorphes, Par cet isomorphisme à une extension avec

$$\forall \alpha, \beta \in K \qquad m(\alpha,\beta) = 0$$

correspond un système $\tau(\alpha)$ de translations non-primitives de la forme

$$\tau(\alpha) = \alpha \circ x - x \qquad \text{où } x \in R^n/Z^n \quad .$$

Salutations amicales de Edgar

Letter Edgar

1967 A letter of Edgar Ascher on non-primitive translations

Cristallographie algébrique.

Je commence par la théorie non orientée. Un groupe d'espace (non orienté) est un groupe G qui possède au moins un sous-groupe U jouissant des propriétés suivantes :

1) U est abélien libre (de dimension $n < \infty$)
2) U est abélien maximal
3) U est normal dans G
4) G/U est fini

Théorème 1. Le sous-groupe U est normal abélien libre maximal, c'est-à-dire contient tout sous-groupe normal abélien libre de G.

Démonstration. Soit V un sous-groupe normal abélien libre de G et soit v un élément de V. Il faut démontrer que v est un élément de U ou encore puisque U est abélien maximal dans G que pour tout élément u de U, $uv = vu$. Soient donc $u \in U$ et $v \in V$ et appelons $v^{-1}u^{-1}vu$ ω. Puisque G/U est fini, il existe un nombre k avec v^k dans U. On a $u^{-1}vu = v\omega$, donc $(u^{-1}vu)^k = (v\omega)^k$. Mais $(u^{-1}vu)^k = u^{-1}v^k u = v^k$ puisque U est abélien. Ainsi $v^k = (v\omega)^k$, mais v et $v\omega = u^{-1}vu$ sont dans V (puisque V est normal) et V est abélien libre, donc $v = v\omega$ et $\omega = e$; donc $v^{-1}u^{-1}vu = e$ ou $vu = uv$.

Corollaire 2. Le sous-groupe U est unique.

Lecture notes 1960 Lecture notes on Space groups by André Michel, Battelle, Geneva

PROPERTIES OF

SHUBNIKOV POINT GROUPS

(PART ONE)

by

Edgar Ascher

A contribution to a

work by

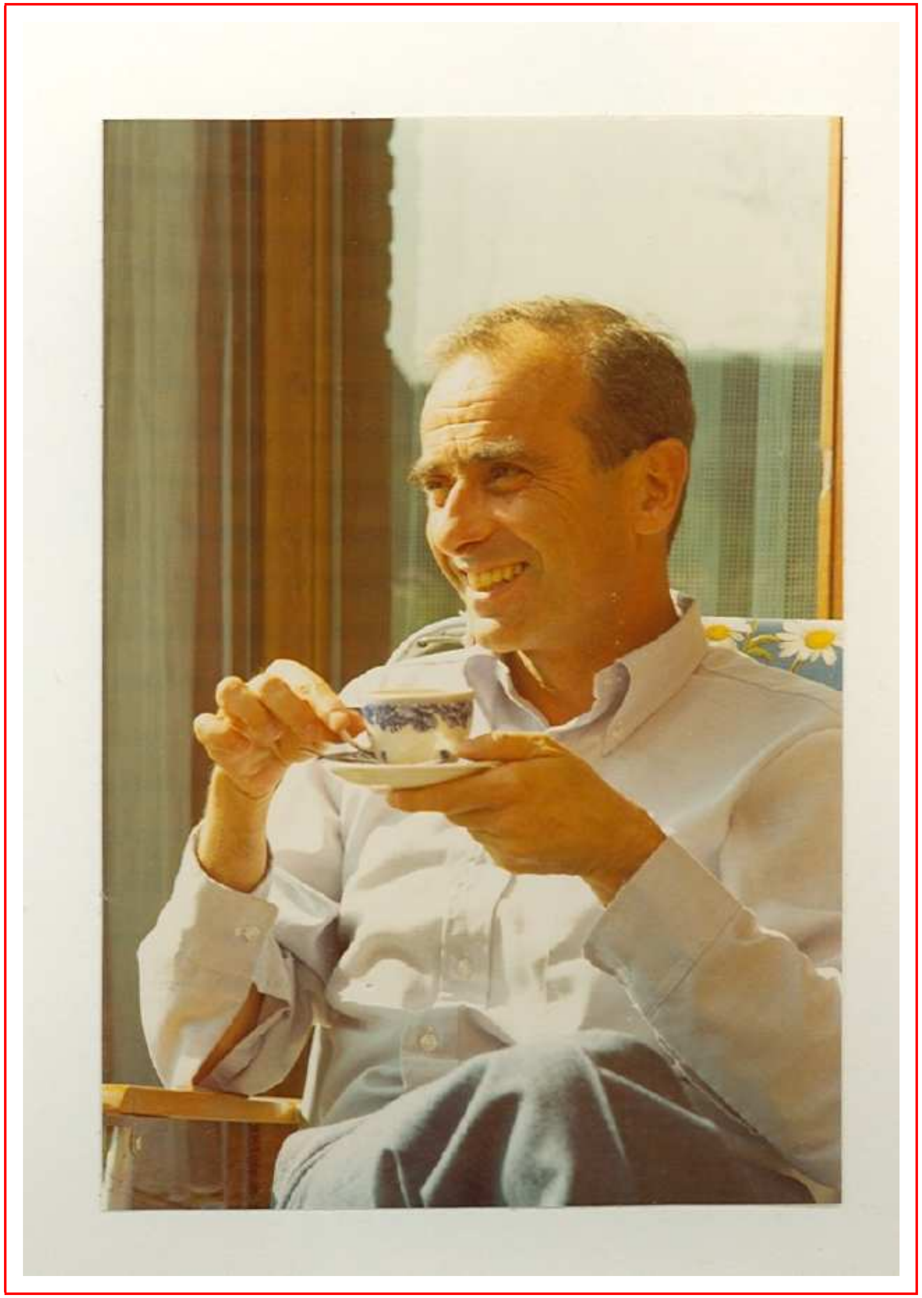
E. Ascher and A.G.M. Janner

BATTELLE INSTITUTE
Advanced Studies Center
Geneva-Switzerland

Report

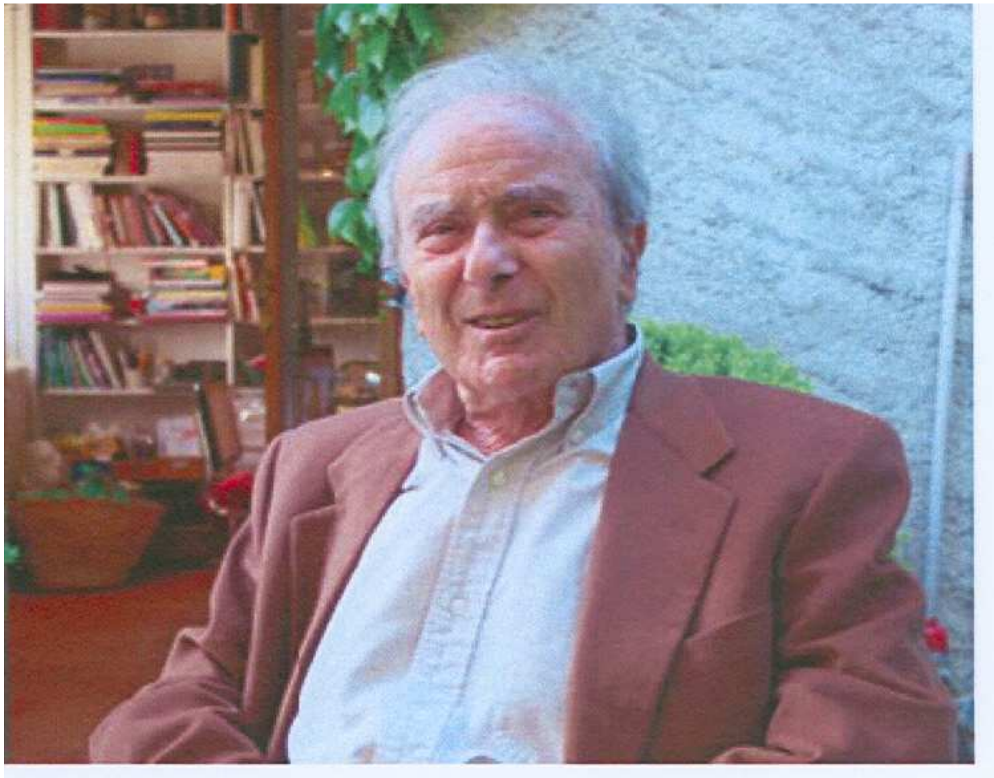
1965 Front page of a typical Battelle report

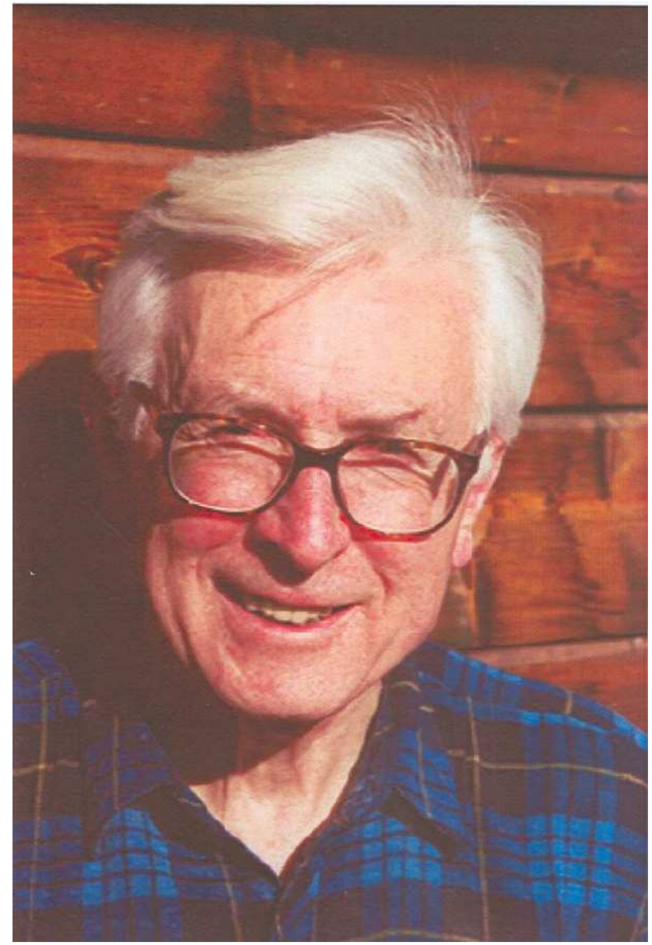
1971 Edgar and Corinna Ascher Nijmegen



1973 Edgar Ascher

Edgar 1973





Edgar Ascher 2000 Hans Schmid