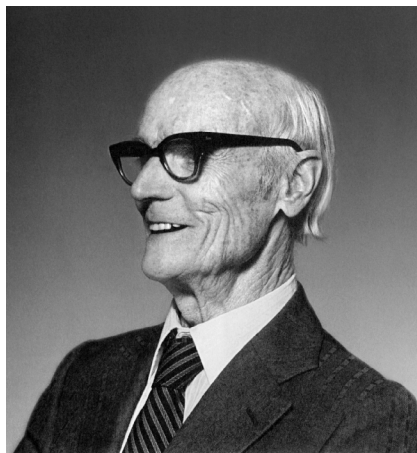


# Coxetering Crystals

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*A reader whose standpoint is more severely practical may take comfort in Lobatschewsky's assertion that 'there is no branch of mathematics, however abstract, which may not some day be applied to phenomena of the real world.'* [Regular Polytopes, p. vi]



Donald Coxeter, 1993,  
photograph by Stan Sherer

"Applied mathematics" is not a phrase "Coxeter" evokes in anyone's mind, and probably never in his own. But H.S.M. Coxeter appreciated -- indeed, delighted in -- the symbiotic relation between polytopes and crystals. His classic *Regular Polytopes* is indispensable for the mathematical study of crystals, never more than now.<sup>1</sup>

Coxeter also appreciated and delighted in the symbiotic relation between models -- the kind you can pick up, turn over, study from different perspectives -- and their abstract descriptions. (Or do the models describe the abstractions?) Eggs and chickens aside, crystallography is a mathematical gold mine in any dimension, and Coxeter delighted in this too.

Regular polytopes and tessellations in four, five,  $n$  dimensions: *we can never fully comprehend them by direct observation*, Coxeter wrote. *In attempting to do so, however, we seem to peep through a chink in the wall of our physical limitations, into a new world of dazzling beauty.* A beauty so dazzling we must study its shadows, and he taught us how.

I hope, in these eight pages, to justify these statements. That's why I've written this paper in the form of a picture booklet. Look before you read. The pictures come first. All the rest -- quotations from *Regular Polytopes* and Coxeter's world-wide correspondence, my supplementary remarks -- is commentary.

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<sup>1</sup> H.S.M. Coxeter, *Regular Polytopes*, Dover Publications, 3rd edition, 1973.

## Crystals and Polyhedra

*The foundations for our subject were laid by the Greeks . . . but all the more elaborate developments are less than a century old. This revival of interest was partly due to the discovery that many polyhedra occur in nature as crystals. [Regular Polytopes, p. vi]*

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Fig. 48.

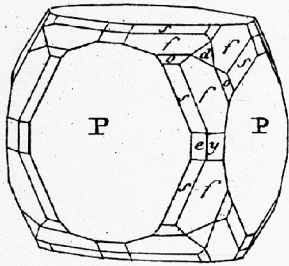


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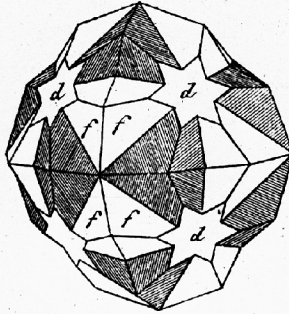


Fig. 50.

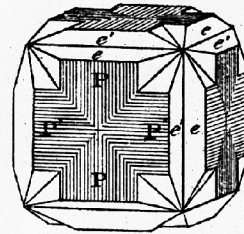


Fig. 51.

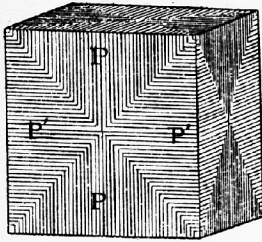


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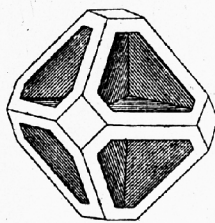


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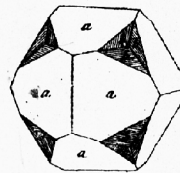


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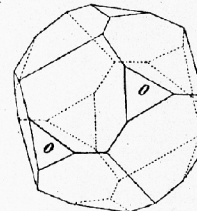


Fig. 55.

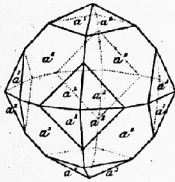


Fig. 56.

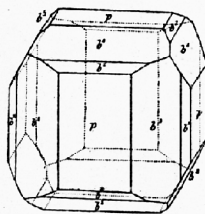


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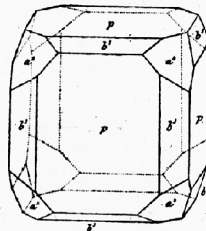


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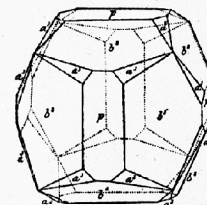


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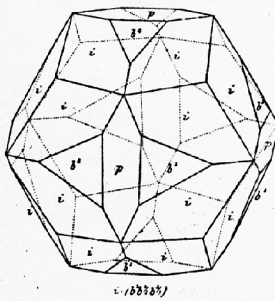


Fig. 60.

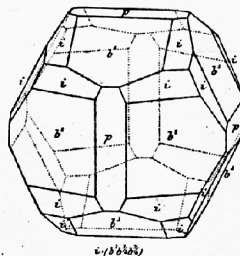
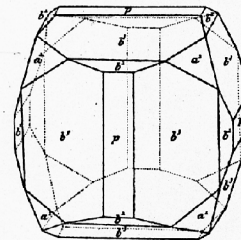


Fig. 61.



Many polyhedra do occur in nature as crystals, and many crystals have polyhedral forms. A century ago, mineralogists pored over drawings like those you see here, 14 of the 23,606 crystal forms in Viktor Goldschmidt's nine-volume *Atlas der Krystallformen*.<sup>2</sup>

Why all this painstaking labor, this manic detail? Not for art's sake, nor for geometry's sake, but for science's. Long before recorded history, people marveled at crystals and their striking geometric shapes and wondered how and why. Even fragments of shattered crystals have smooth flat faces, unlike glass. Early in the 19th century, René Just Haüy, a French mineralogist, proposed a how and why: crystals are stacks of sub-visible bricks.<sup>3</sup> The crystallographer's job, then, was to deduce, for each polyhedral crystal, the shape of its brick – its height, width, depth, and interfacial angles. Hence the study of form.

Goldschmidt's labor of love was obsolete before the first volume appeared. The discovery, in 1912, that X-rays are diffracted by crystals unlocked the mysteries of the solid state.<sup>4</sup> The positions of atoms in any crystal, polyhedral or otherwise, could be deduced from the scattered rays. Haüy's hypothesis became history, but diffraction's overnight success rested squarely on his notion that a crystal's building blocks – atoms, molecules, whatever – line up in rows and columns. Tilings, polyhedra and symmetry groups remained in the crystallographer's toolbox.

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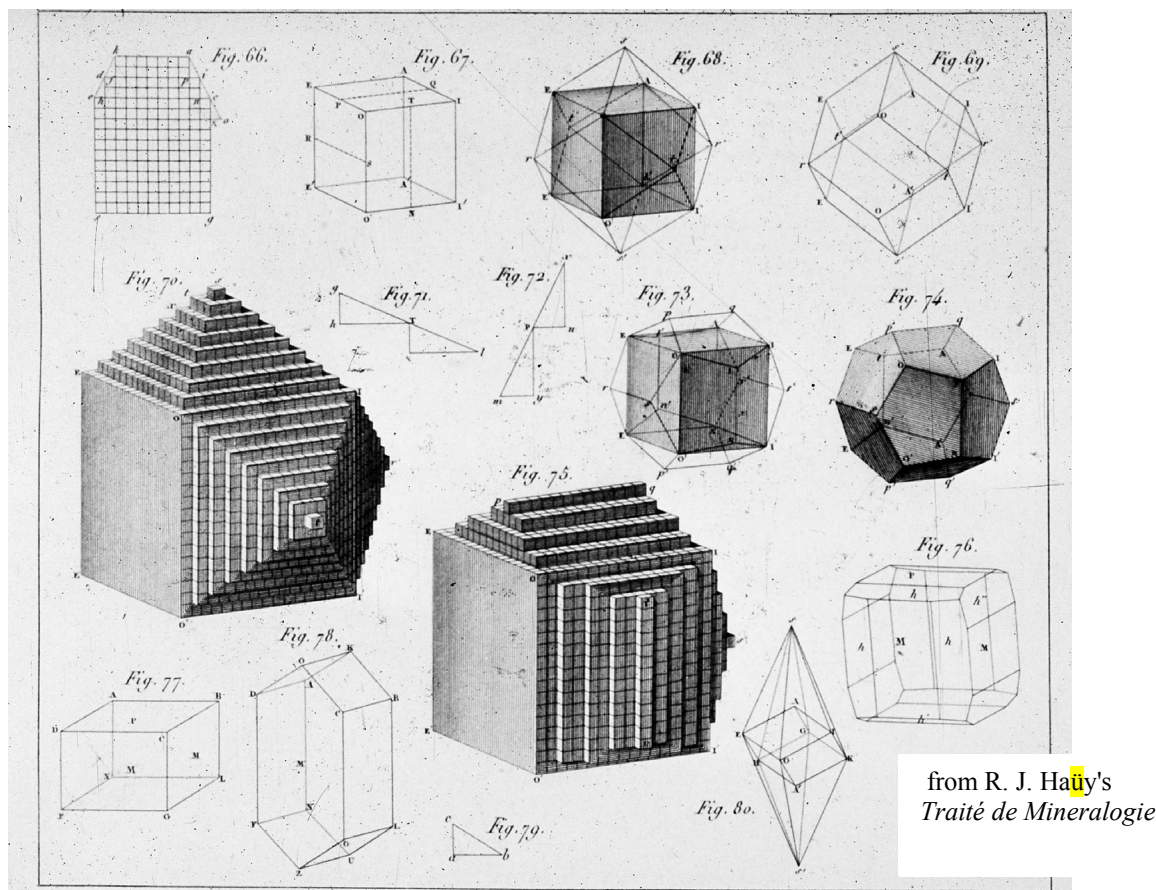
<sup>2</sup> V. Goldschmidt, *Atlas der Krystallformen*, Munich, 9 volumes, 1913 - 1923.

<sup>3</sup> R. J. Haüy, *Traite de Mineralogie*, Paris, 1822.

<sup>4</sup> Max von Laue received the Nobel Prize in Physics for this discovery in 1914.

## The Crystallographic Restriction

*There is a law of symmetry which prohibits the inanimate occurrence of any pentagonal figure, such as the regular dodecahedron. The two more complicated regular solids cannot form crystals, but need the spark of life for their natural occurrence. [Regular Polytopes, p. 13]*



In this drawing, from *Traité de Mineralogie*, Haüy shows how two different polyhedral crystal forms can be approximated by stacking bricks of the same size and shape. Both forms display the symmetries of the stacking pattern. The difference in the exterior forms is literally superficial.

Look closely at the polyhedron in the middle on the right, a common form of the mineral pyrite. Although the "pyritohedron" has twelve pentagonal faces, it's not a *regular* pentagonal dodecahedron (see *Regular Polytopes*): one edge in each of its pentagons is longer than the other four. According to Haüy, crystal faces *can't* be regular pentagons. Haüy's brick theory implies that the vertices of every crystal are rational triples in the coordinate system defined by its brick. A pyritohedral stack is shown in lower center.

Mineralogists call this the "Law of Rational Indices." Regular pentagons, and hence regular pentagonal dodecahedra, don't have rational vertices in *any* coordinate system. Nor do regular  $n$ -gons for any  $n$  greater than 6. In symmetry group language, Haüy's law becomes The Crystallographic Restriction:<sup>5</sup>

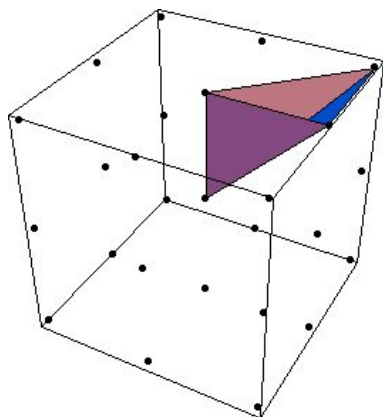
*If a discrete group of displacements in the plane has more than one centre of rotation, then the only rotations that can occur are 2-fold, 3-fold, 4-fold, and 6-fold.*

The regular dodecahedron and icosahedron are outlaws in the crystal kingdom.

<sup>5</sup> *Regular Polytopes*, p. 63

## Kaleidoscopes and honeycombs

*A three-dimensional honeycomb (or solid tessellation) is an infinite set of polyhedra fitting together to fill all space just once, so that every face of each polyhedron belongs to one other polyhedron. . . Three dimensional honeycombs help us to understand the arrangement of atoms in a crystal. [Regular Polytopes, p. 74.]*



left: repeated reflections in a cone of three mirrors with interior angles  $\pi/4$ ,  $\pi/4$ , and  $\pi/2$  generate a three-dimensional pattern with cubic symmetry;

below: Coxeter's elegant graphical notation for the group generated by these reflections.



The kaleidoscope, introduced in 1818, “very quickly became popular . . . no fewer than two hundred thousand instruments were sold in London and Paris in three months.”<sup>6</sup> This grieved its inventor, the Scottish physicist David Brewster, for most of these “instruments” were patent-infringements and – just as sadly – “out of this immense number there were perhaps not one thousand constructed on scientific principles.” Brewster expected the kaleidoscope would be, first and foremost, a tool for industrial design, and only secondarily an “instrument of rational amusement.” But a toy it remained for 116 years, until Coxeter gave it gravitas.<sup>7</sup>

While crystallographers argued over Haüy’s bricks (are they solid? or fictional containers for possibly fictional molecules?), mathematicians analyzed the arrangements, not the arranged.<sup>8</sup> In *Regular Polytopes*, Coxeter described highly symmetrical tessellations in the plane and in three-space, and in the beyond. He’s best known for his study of groups generated by reflections: the analysis, classification, and systematization of tessellations generated by reflections in any dimension. Brewster himself had constructed a 3-D kaleidoscope (the mirrors above generate a cubic pattern), but Coxeter generalized the kaleidoscope beyond Brewster’s fondest dreams.

In Coxeter’s famous graphical notation for these groups, the generating mirrors are represented by dots which are joined by line segments unless the mirrors are perpendicular. Since adjacent mirrors generate a circular pattern with a whole number of mirror-symmetric images, the angles must be  $\pi/p$ , where  $p$  is an integer greater than one. In Coxeter graphs, a line is labeled by that integer if  $p > 3$ . Hence the 4 in the graph above. If we added a fourth mirror to complete the tetrahedron, the pattern would be crystallographic: infinite in all directions.

<sup>6</sup> Quoted by David Brewster in *The Kaleidoscope, its history, theory, and construction*, reprinted by Van Cort Publications, Holyoke, MA, 1987.

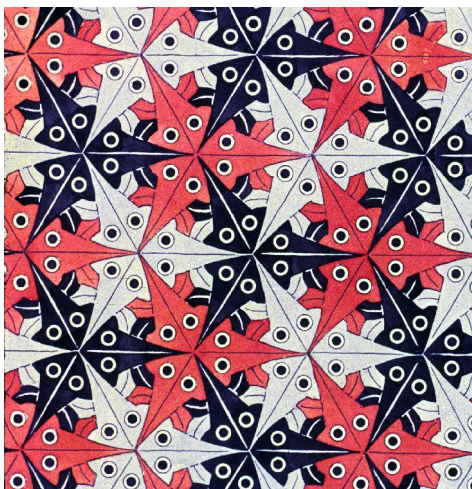
<sup>7</sup> H.S.M. Coxeter, “Discrete groups generated by reflections,” *Annals of Mathematics*, 35, 1934, 588-621.

<sup>8</sup> As Arthur Schönflies put it, “within the fundamental domain the crystallographer may do as he likes.”



## Color Symmetry

*The problem of systematically coloring periodic patterns has interested textile designers, artists, and crystallographers since 1935. The classification of possible procedures has been seen to depend on space groups and their subgroups and factor groups. Crystallographers naturally worked in Euclidean 3-space before generalizing to two, and then four, dimensions.<sup>9</sup>*



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Crystallographers and mathematicians discovered the mathematical drawings and prints of M. C. Escher in the 1950s. His tessellations soon appeared in their monographs and texts, giving life to group theory and to the tedious study of crystalline arrangements. In Escher's kaleidoscopic tessellation above, which illustrates the plane crystallographic group  $p31m$ , the mirrors bisect the fish to form equilateral triangles enclosing a half-fish of each color.

Escher designed this pattern before he met Coxeter. Later, Coxeter sent him other mathematical ideas which Escher converted to art, a process he called “coxetering.”<sup>10</sup>

Look closely: there's more than mirrors here. The red fish (and the black and the gray) are arranged in hexagonal rings. Except for their colors, the three sets of rings are congruent. The fish of each color correspond to subgroups of the tessellation's symmetry group, which permutes them. In other words, this pattern has *color symmetry*. Crystallographers use color symmetry theory to describe the positions of the different kinds of atoms in a single crystal, like the checkerboard pattern of Na and Cl atoms in salt.

Coxeter was intrigued by color groups; we corresponded intensively about them for a few years. He was particularly interested in the problem of notation, and developed symbols for color groups of certain types.

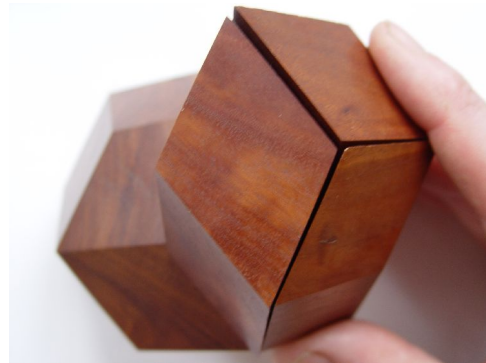
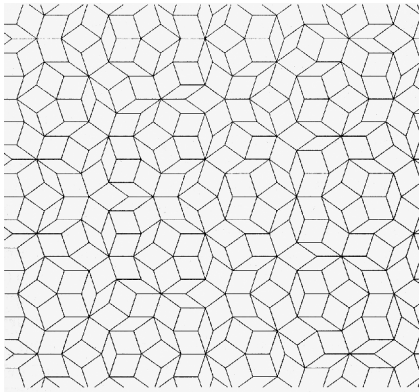
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<sup>9</sup> H. S. M Coxeter, "A Simple Introduction to Colored Symmetry," *International Journal of Quantum Chemistry*, 31, 1987, 455-461.

<sup>10</sup> See D. Schattschneider, “Coxeter and the Artists: two-way inspiration”, *The Coxeter Legacy*, *Fields Communications* v. 46, Amer. Math. Soc., Providence, 2005.

## Nonperiodic honeycombs

*Dear Dr. Miyazaki, What I would be interested to know is whether rhombohedra fill space in a manner that is essentially non-periodic (in the sense that no honeycomb composed of these particular bricks can have a translation into itself). If the answer is yes, we would have here a very nice 3-dimensional analogue for the non-periodic tilings of Roger Penrose. [H.S.M. Coxeter to Kojo Miyazaki, April 22, 1977.]*



left: a portion of a Penrose tilings by rhombs; right: models of A6 and O6 made by A. G. Bomford

Like Hány's arrays, kaleidoscope tilings are periodic: they repeat by translations, or shifts. Penrose tilings are nonperiodic: no tiling built with Penrose tiles repeats by translation in any direction. In the version shown above left, the Penrose tiles are rhombs with acute angles  $72^\circ$  and  $36^\circ$ , constrained by "matching rules" for putting them together. Though these rules forbid translation, configurations do repeat – but you can't predict just where. All seven "legal" arrangements of Penrose rhombs around a vertex occur again and again in the fragment above .

Like fractals, Penrose tilings repeat on every scale. Many of the tilings' remarkable features follow from this property, including their nonperiodicity. Coxeter was intrigued by the possibility of a three-dimensional analogue and proposed the two golden rhombohedra, A6 and O6, as tiles.<sup>11</sup> The dihedral angles of A6 are the polygonal angles of the thick Penrose rhomb, and those of O6 are those of the thin. He hoped to show, first, that these rhombohedra can build tilings that repeat on every scale, and second, that matching rules could be found to enforce it.

Earlier, in *Regular Polytopes*, Coxeter had shown that 10 A6s and 10 O6s make a Kepler triacontahedron, K30. Could that construction be repeated on larger scales *ad infinitum*?

A friend A.G. Bomford, an Australian engineer, made the wooden models of A6 and O6 shown above.<sup>12</sup> The blocks are handsome and smooth, but difficult to stick together. Thin tape worked well, up to a point, but even the thinnest tape creates cascading gaps eventually. Coxeter finally gave up, pleading with Bomford, *I don't have the time or patience to try it myself, so please don't embarrass me by sending the necessary pieces!*

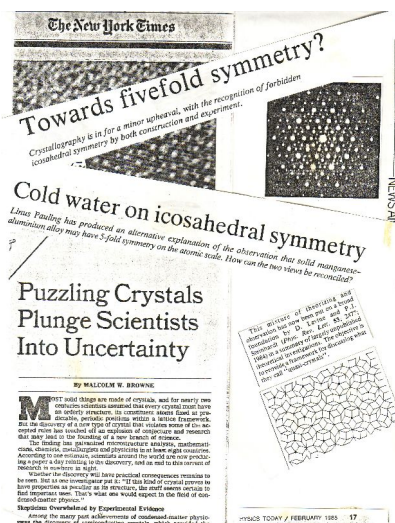
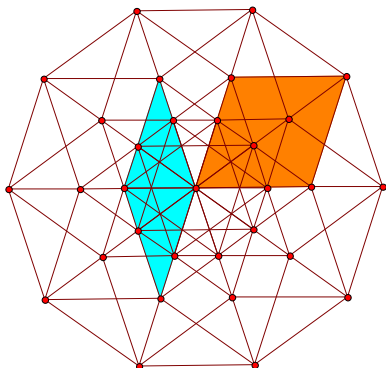
<sup>11</sup> A polyhedron is golden if its faces are golden rhombs; a rhombus is golden if the lengths of its diagonals stand in the golden ratio.

<sup>12</sup> Richard Bomford has kindly photographed his father's models for this article.

## Icosahedral crystals

Dear Dr. Nelson, Thank you for the reprints from 'Science' and the 'New York Times' about quasi-crystals. They reached me the next day after your lecture in Toronto. They reminded me of many things I had been thinking about in former times. [H.S.M Coxeter to David Nelson, January 22, 1986.]

the 2-dimensional faces of a 5-dimensional cube project to the Penrose rhombs.



In 1984, solid state scientists – and mathematicians – were stunned by the announcement of the impossible: crystals with *bona fide* icosahedral symmetry had been grown in a laboratory! Not only did the forms of these crystal have outlaw symmetry, their diffraction patterns did too. But then so must their atomic patterns, at least statistically. *That's impossible, isn't it?* No, it's not: no law of nature, nor of mechanics, says atoms in crystals must line up periodically. The Crystallographic Restriction isn't a theorem about crystals and never was. Like Haüy's Law of Rational Indices, it's a theorem about arrays, the standard mathematical *model* for crystals.

How, then, to envision these new atomic patterns? Suggestions lay waiting. In 1981, Alan Mackay, a far-sighted crystallographer, had punched the vertices of a Penrose tiling into a metal plate and use this to diffract visible light. His optical diffraction patterns strongly resembled the icosahedral X-ray patterns: perhaps the new crystals were 3-D Penrose tilings!<sup>13</sup> That same year, N.G. de Bruijn showed that Penrose tilings of the plane are projections of sections of the cubic tessellation of 5-dimensional space.<sup>14</sup> Indeed – see *Regular Polytopes*, p. 244 – the 2-dimensional faces of a 5-dimensional cube project to the Penrose rhombs. De Bruijn's reformulation opened the door, or the lid, to non-periodic tilings in any dimension.

*I find it fascinating that all this nice geometry has physical applications despite the disclaimers in those textbooks which you exhibited, and my own rash assertion (RP, p 13) that 'the 2 more complicated regular solids need the spark of life for their natural occurrence'!* Coxeter concluded his letter to Nelson.

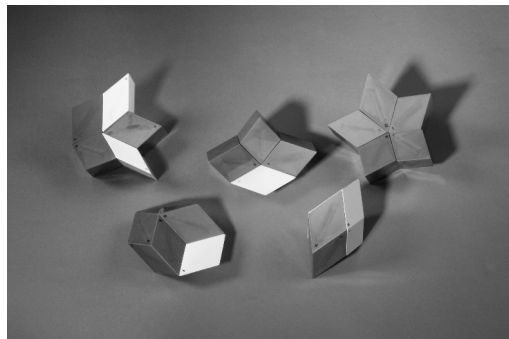
<sup>13</sup> A. M. Mackay, De nive quinquangula - On the pentagonal snowflake, *Sov. Phys. Crystallogr.*, 26, 1981, 517-522

<sup>14</sup> N. G. de Bruijn, Algebraic theory of Penrose's non-periodic tilings of the plane, *Kon. NederL Akad. Wetensch. Proc. Ser.*, A84, 1981, 39-52 and 53-66.



## Nonperiodic honeycombs, continuing . . .

*Dear Mr. Ammann, I am much interested in your 1976 discovery of a three dimensional analogue of Penrose's nonperiodic tilings, namely a packing of acute and obtuse rhombohedra whose faces are golden rhombs. . . Would it be possible to decorate the rhombohedra with pits and pimples so as to be the infinite assembly essentially nonperiodic?* [H. S. M. Coxeter to Robert Ammann, February 19, 1986]



Five "Rhombos" block configurations that obey Ammann's matching rules. Photograph by Stan Sherer.

The icosahedral crystals rekindled Coxeter's interest in 3-D Penrose tiles. Robert Ammann, an amateur geometer, had found matching rules (x's for bumps, o's for dents, the former fitting into the latter) for the golden rhombohedra.<sup>15</sup> As this photograph of five rule-abiding configurations suggests, Ammann's rules closely mimicked Penrose's. But do his tilings repeat on all scales?

*I agree that twenty such rhombohedra (10 acute and 10 obtuse) can be assembled to form a triacontahedron, Coxeter continued. I am anxious to know whether a triacontahedron K30 could possibly be surrounded by 70 A6s and 70 O6s in such a way as to preserve icosahedral (rotatory) symmetry and make a big K30 (of edge 2).*

Possibilities for Coxetering quasicrystals improved dramatically in 1993, when Michael Longuet-Higgins presented Coxeter with prototypes of his "Rhombos" blocks. These plastic golden rhombohedra – shown above – have magnetized faces: no sticky tape needed. A decade later, Longuet-Higgins's "big K30 (of edge 2)" graced a cover of *The Mathematical Intelligencer*.<sup>16</sup> This construction, repeated *ad infinitum*, generates a nonperiodic tessellation of three-dimensional space, but not by Ammann's rules. Evidently, it's impossible to decorate the rhombohedra to make Longuet-Higgins's construction *essentially* nonperiodic. Coxeter's questions remain open -- as does the relation of any Penrose-type tiling to real crystal structure.<sup>17</sup>

Coxeter's greatest joy, I think, was the search itself. He delighted in the beauty of the golden rhombohedra's fertile, three-way, symbiotic interactions: a quasicrystallographic tool, a geometric model, and perhaps especially a wedge for widening the chink in the wall of our physical limitations. *I find your new paper fascinating*, he wrote to Longuet-Higgins, *an ideal rebuttal to the anti-Platonists who claim that mathematics is a human invention like poetry*.<sup>18</sup>

<sup>15</sup> M. Senechal, "The Mysterious Mr. Amman," *The Mathematical Intelligencer*, v. 26, no. 4, 2004, 10-21.

<sup>16</sup> Michael Longuet-Higgins, "Nested Triacontahedral Shells, or how to grow a quasicrystal," *The Mathematical Intelligencer*, v. 25, no. 2, 2003, 25-43.

<sup>17</sup> M. Senechal, "Donald and the Golden Rhombohedra," *The Coxeter Legacy*, Fields Communications v. 46, Amer. Math. Soc., Providence, 2005.

<sup>18</sup> May 6, 2001, Coxeterhsm@aol.com to mlonguet@uscd.edu.