

Periodic minimal surfaces of cubic symmetry

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A survey of cubic minimal surfaces is presented, based on the concept of fundamental surface patches and their relation to the asymmetric units of the space groups. The software Surface Evolver has been used to test for stability and to produce graphic displays. Particular emphasis is given to those surfaces that can be generated by a finite piece bounded by straight lines. Some new varieties have been found and a systematic nomenclature is introduced, which provides a symbol (a 'gene') for each triply-periodic minimal surface that specifies the surface unambiguously.

'An experiment is a question which we ask of Nature, who is always ready to give a correct answer, provided we ask properly, that is, provided we arrange a proper experiment.'

C. V. Boys, *Soap Bubbles*, 1890

The Society for Promoting Christian Knowledge, London

WHEN we consider growth and form, morphogenesis, metamorphosis and shapes generally, in our three-dimensional space, it is necessary to have a vocabulary¹. Since classical times, the fundamental elements have traditionally been the five Platonic solids² (the cube, octahedron, tetrahedron, icosahedron and dodecahedron), along with the sphere. The 15 books of Euclid culminate in a description of how to inscribe each of the Platonic solids in a cube or in a sphere.

In our culture, the cube dominates. Hugh Kenner, in his essay on Buckminster Fuller wrote: 'Each of us carries in his mind a phantom cube, by which to estimate the orthodoxy of whatever we encounter in the world of space'³. It is not an accident that we prefer the cube because its three sets of edges are orthogonal, that is, it can be changed in one direction without affecting the others. Descartes invented the Cartesian coordinate system, the x , y , z coordinates, which permitted the representation of geometry in space as an algebra of symbols.

However, especially for biological purposes, we need to consider curved surfaces. The sphere is important; typically, it occurs in bubbles, where the physical condition is that the content should be the maximum for a given surface area; but it is only the simplest of all curved surfaces. Life begins with the cell or micelle, where a limited number of lipid molecules form a bilayer which

encloses a volume and makes the all-important distinction between inside and outside. Next, there may be aggregates of cells, foam, where a volume is divided into separate regions by curved partitions. Natural foams are usually irregular with a spread of cell shapes, but crystallography has provided the theory of idealized foams, where all the cells are identical.

Crystallography has supplied the theory for geometry of the regular periodic arrangements of molecules in space. In crystals, there are asymmetric 'motifs', all identically situated, repeated infinitely in three non-coplanar directions. It was a triumph of 19th-century theory to discover that there are exactly 230 different symmetries of such arrangements – the 230 space groups⁴. Geometrically, the asymmetric unit may be seen as a simple convex polyhedron containing the asymmetric motif, which is repeated by the symmetry operations to fill all space. By curving the faces of such a polyhedron, it is possible to make a 3D jigsaw puzzle piece such that many copies of such a piece will fit together in only one way to fill space periodically, with the symmetry of any one of the 230 space groups⁵. Each of the 230 space groups can be specified by the shape of such a piece.

We are concerned here to fit elements of surface – patches – into these units, so that the surface becomes continuous through all space, dividing it into two, not necessarily equal, sub-spaces by a non-self-intersecting two-sided surface. The elements of symmetry act like a generalized kaleidoscope on the motif. We thus generate two-dimensional manifolds of complex topology and non-Euclidean metric embedded in three-dimensional space.

Here, we will confine ourselves to the cubic space groups, since no parameters are involved and the surfaces of this class are of the greatest complexity and interest. These surfaces are invariant structures, comparable to the five regular solids, in terms of which many naturally-occurring structures can be understood and described^{6–9}. For example, in the structure of sodalite (a mineral zeolite used in water-softening), the silicate cage lies on the P-surface.

Coxeter and Petrie, when still undergraduates, discovered a number of infinite polyhedra¹⁰ (the sodalite network was one), closely related to these periodic minimal surfaces (PMS) by relaxing the condition that polyhedra had to be convex. Some of the PMS can be obtained by curving the faces of such polyhedra and by connecting them with catenoidal tunnels.

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Minimal surfaces

Surfaces whose mean curvature H is everywhere zero are *minimal surfaces* – any sufficiently small patch cut from a minimal surface has the least area of all surface patches with the same boundary. The shapes taken by soap films are minimal surfaces. The catenoid, the surface of revolution of a catenary, is a simple example. It is the shape taken up by a soap film hung between two circular rings. If the rings are far apart, the only solution is that of two isolated flat films covering each ring. If the rings are close together, then there are two catenoidal solutions, one stable and realizable as an actual soap-film, and the other unstable. The first is almost a cylinder stretching directly from one ring to the other and the second also stretches from one ring to the other, but has a waist strongly pinched into a much smaller diameter. Both have $H = 0$, but the first has a smaller area. As the rings are moved apart from each other, the two surfaces approach each other and at a critical distance they become identical. For greater separations, there is no catenoid. Similar phenomena are to be found for more complicated minimal surfaces; catenoid-like ‘tunnels’ are to be found in most PMS. A variant of the catenoid is a minimal surface hung between two square frames, which occurs in the structure of the P-surface. Varying the distance between the two squares corresponds to a sequence of surfaces with tetragonal symmetry.

The triply periodic minimal surfaces (TPMS) are particularly fascinating. A TPMS is infinitely extending, has one of the crystallographic space groups as its symmetry group and, if it has no self-intersections, it partitions space into two labyrinthine regions. Its topology is characterized by two interpenetrating networks – its ‘labyrinth graphs’.

The first TPMS to be discovered and investigated was reported by Schwarz in 1856 (ref. 11). He considered a soap-film across a quadrilateral frame, the edges of which are four of the six edges of a regular tetrahedron and realized that such a surface could be smoothly continued by joining the pieces edge to edge, the edges becoming two-fold [diad] axes of symmetry of the resulting infinite object. Six such quadrilaterals occur in a cubic unit cell of space group $Pn\bar{3}m$. However, if the two sides of the surface are coloured differently, then the cells alternate in colour, the repeat distance is doubled and the space group becomes $Fd\bar{3}m$. The surface is known as the D-surface, because its labyrinth graphs are four-connected diamond networks – the surface can be obtained by taking the structure of diamond, where the C atoms are tetrahedrally connected, and inflating the bonds until the two sub-spaces become equal. It can also be visualized as the surface separating the two distinct networks in the ‘double diamond structure’ of cuprite Cu_2O . By an ingenious application of a formula of Weierstrass, Schwarz was able to obtain an analytic expression for the D-surface, and also

for the P-surface, whose labyrinth graphs are networks consisting of the vertices and edges of a primitive cubic lattice. His student Neovius discovered $C(P)$ – the ‘complement’ of P, so-called because P and $C(P)$ have the same symmetry group¹².

The next development in TPMS did not take place until the 1960s, when Schoen¹³ investigated for NASA whether surfaces of this type might be of use as space structures, and found more than a dozen new examples. Those surfaces with cubic symmetry are called (following Schoen’s rather eccentric notation) IWP, FRD, OCTO, $C(D)$ and G (‘the gyroid’).

An intensive search for new possibilities was taken up by Fischer and Koch from 1987. In a remarkable sequence of papers^{14–21}, they systematically investigated the various ways in which frameworks of diad axes of the space groups can be spanned by minimal surfaces. The two labyrinths of a TPMS obtained in this way are necessarily congruent, since a two-fold rotation about a diad axis embedded in the surface interchanges the two sides of the surface. Triply periodic surfaces with congruent labyrinths are called *balance* surfaces. Their symmetry properties are described by *two* space groups: G, the symmetry of the surface, and H (a subgroup of G of index 2), the symmetry of a single labyrinth. The gyroid is unique; it is a balance surface with no embedded diad axes – the transformations that interchange the labyrinths are inversion centres lying on the surface. Koch and Fischer listed exhaustively all pairs of space groups G/H which might have associated balance surfaces and found a large number of new triply periodic minimal balance surfaces (TPMBS). Those with cubic symmetry are called S, $C(Y)$, $^{\pm}Y$, $C(^{\pm}Y)$, $C(P)/H$, $C(D)/H$ and $C(Y)/H$.

In 1990, Gozdz and Holyst²² discovered two more cubic TPMS which they called BFY (‘the Butterfly’) and CPD. Karcher and Polthier²³ indicated how in certain cases more complicated variants of known surfaces could arise by inserting extra tunnels in their labyrinths.

It has now become apparent that the nomenclature for minimal surfaces is getting out of hand. What is needed is a way of naming a surface so that the structure of the name reveals unambiguously which surface is being referred to – a system analogous to the Hermann–Mauguin symbols for space groups, or the ‘inorganic gene’ that employs Delaney–Dress symbols to specify triply periodic networks²⁴.

Some minimal surfaces can be given exact parametric expression (x, y, z coordinates of all points in the surface expressed in terms of two parameters); but in the cases where this can be done, the expressions are complicated and involve elliptic functions. Weierstrass provided the algebraic method of obtaining these functions^{25–29}. The most effective method is to use the engineering methods of finite element analysis as provided by Brakke³⁰ in a remarkable publicly available program called the Surface Evolver, which will minimize either surface area or the

integral of H^2 . Some of the seemingly plausible possibilities for new minimal surfaces turn out to be unstable when ‘evolved’ by Surface Evolver; as the area per unit volume decreases, a critical configuration arises, indicating that the surface collapses catastrophically to one with a different topology. In such cases, no *minimal* surface exists with the specified symmetry and topology. Employing the ‘curvature-squared’ option in these cases leads to a stable configuration which minimizes the integral of H^2 . Surface Evolver can thus deal readily with the class of unstable surfaces. The answers are physically rather than mathematically conclusive, but there are tests for the stability, or otherwise, of a solution. Having plotted a surface, it can then be more simply expressed as the surface for which the sum of various Fourier terms is zero, i.e., as a nodal surface. The simplest example is the P-surface which, to a first approximation, can be described as the surface for which $\cos(x) + \cos(y) + \cos(z) = 0$. The exact G-surface is very close to the nodal surface $\sin(x)\cos(y) + \sin(y)\cos(z) + \sin(z)\cos(x) = 0$. The programming system Mathematica has provision for plotting such surfaces most conveniently, and von Schnering and Nesper have listed a number of useful expressions³¹. The Fourier terms correspond to structure-factor amplitudes and are to be found tabulated in *The International Tables for Crystallography*⁴.

Fundamental units and surface patches

A ‘fundamental region’ or ‘asymmetric unit’ of a given space group is a polyhedron which, when copied by applying all the transformations of the group, produces a *tiling* of space, such that the only transformation of the group that leaves a tile invariant is the identity. *The International Tables for Crystallography* lists the vertices and faces of a unit for each group. Obviously, the whole group is generated by the set of transformations that relate a unit to the units immediately surrounding it, sharing a face or part of a face. The importance of this concept lies in the fact that an asymmetric unit for a space group G contains a *smallest repeating unit* of any triply periodic structure with symmetry G . A crystal structure is described by giving the positions of atoms in such a unit. Here, we insert into the asymmetric unit of a particular cubic space group, a patch or element of surface of zero mean curvature, which is then repeated round, as in a kaleidoscope, to give a non-self-intersecting surface dividing all space into two regions. Inserting a piece of tube would generate 3D knots or weaves which should, as well as the surfaces, have engineering applications. The patch of surface may be inserted in several different ways and may or may not be capable of refinement, so that its mean curvature should become everywhere zero. A number of configurations may have to be tested to see whether they refine to a TPMS. Some candidates may be-

come stuck in a stable local minimum and others may collapse in various ways.

Description of surfaces: an ‘inorganic gene’

The Delaney–Dress symbol, developed for tiling theory, provides a notation which can be used for enumerating networks. It gives a unique linear symbol to each network and an arbitrary symbol can be identified as corresponding (or not) to a valid network. We shall describe here a method of encoding TPMS. Each such surface can be denoted by a string of symbols – a ‘gene’ – that unambiguously specifies the topology and symmetry of the surface. The symbols we use are the standard Wyckoff letters employed in *The International Tables for Crystallography*. For visualization of the surface denoted by a particular string of Wyckoff letters, an actual picture of the asymmetric unit of the group is necessary. The relevant figures, for the groups we shall encounter, are given in Figure 1. As an introduction to this nomenclature, we illustrate it by means of a few examples of *non*-balanced surfaces.

Figure 2 shows a fundamental region for the group $Pm\bar{3}m$ – a tetrahedron of mirrors. The curvilinear pentagon is a boundary for a fundamental patch of a triply periodic surface. The whole surface is produced by repeating the units by application of the reflections. Clearly, a smooth surface without self intersections must cut the mirror planes orthogonally. The *minimal* surface with this symmetry and topology is unique. It is, in fact, Schoen’s OCTO. It can be uniquely specified by the sequence of Wyckoff positions⁴ around the vertices of the fundamental patch. Thus, OCTO can be denoted by the symbol $(Pm\bar{3}m)hiff^2$.

This symbol specifies the symmetry and the topology of the surface unambiguously. It should be noted, however, that the diad rotation about the axis $x, \frac{1}{4}, \bar{x}$, belonging the supergroup $Im\bar{3}m$ is an automorphism on the group $Pm\bar{3}m$. The asymmetric unit is unchanged, but the Wyckoff labels undergo the permutation $(ab)(cd)(ef)(ij)(kl)$. Therefore, OCTO can alternatively be denoted by $(Pm\bar{3}m)hjei^2$. The symbol strings $hiff^2$ and $hjei^2$ could, of course, be cyclically permuted or written in reverse order. For uniqueness, we adopt the convention of choosing the string that heads the list when all possible strings are listed in alphabetical order.

Figure 3 *a* illustrates a fundamental patch of a surface that may be denoted as $(Pm\bar{3}m)effj$. But the *minimal* surface with this description has higher symmetry, $Im\bar{3}m$, and so should be designated $(Im\bar{3}m)ehih$ (Figure 3 *b*). It is Schoen’s IWP. Observe that the vertex i lies on a ‘free’ diad axis (i.e. a diad axis not lying in a mirror plane), so that hi is *necessarily* followed by a second h . The symbol for IWP may therefore be abridged to $(Im\bar{3}m)ehi$.

Gozdz and Holyst's CPD is $(Pm\bar{3}m)hig^2$, Schoen's FRD is $(Fm\bar{3}m)ef_bgh$ and P,FRD is $(Fm\bar{3}m)ef_bhi^2$. In these latter cases, it is necessary to distinguish two segments of the threefold axis (f) that are inequivalent under the action of the group $(Fm\bar{3}m)$ – that is, ac and bc of Figure 1 *a*, which we denote by f_a and f_b . They are interchanged by the reflection $m^{1/4}_y, z$, which belongs to the supergroup $Pm\bar{3}m$ and induces the permutation $(ab)(hi)$ of Wyckoff labels.

Survey of cubic TPMBS

The various surfaces are extremely difficult to visualize and they may be seen at three levels: (1) the *fundamental patch* associated with an asymmetric unit of the space group – the smallest repeating unit; (2) a structural unit, or *generating patch*, usually bounded by straight lines, which may, for example, be a skew polygon or two skew polygons united by catenoid-like tunnels or a set of skew

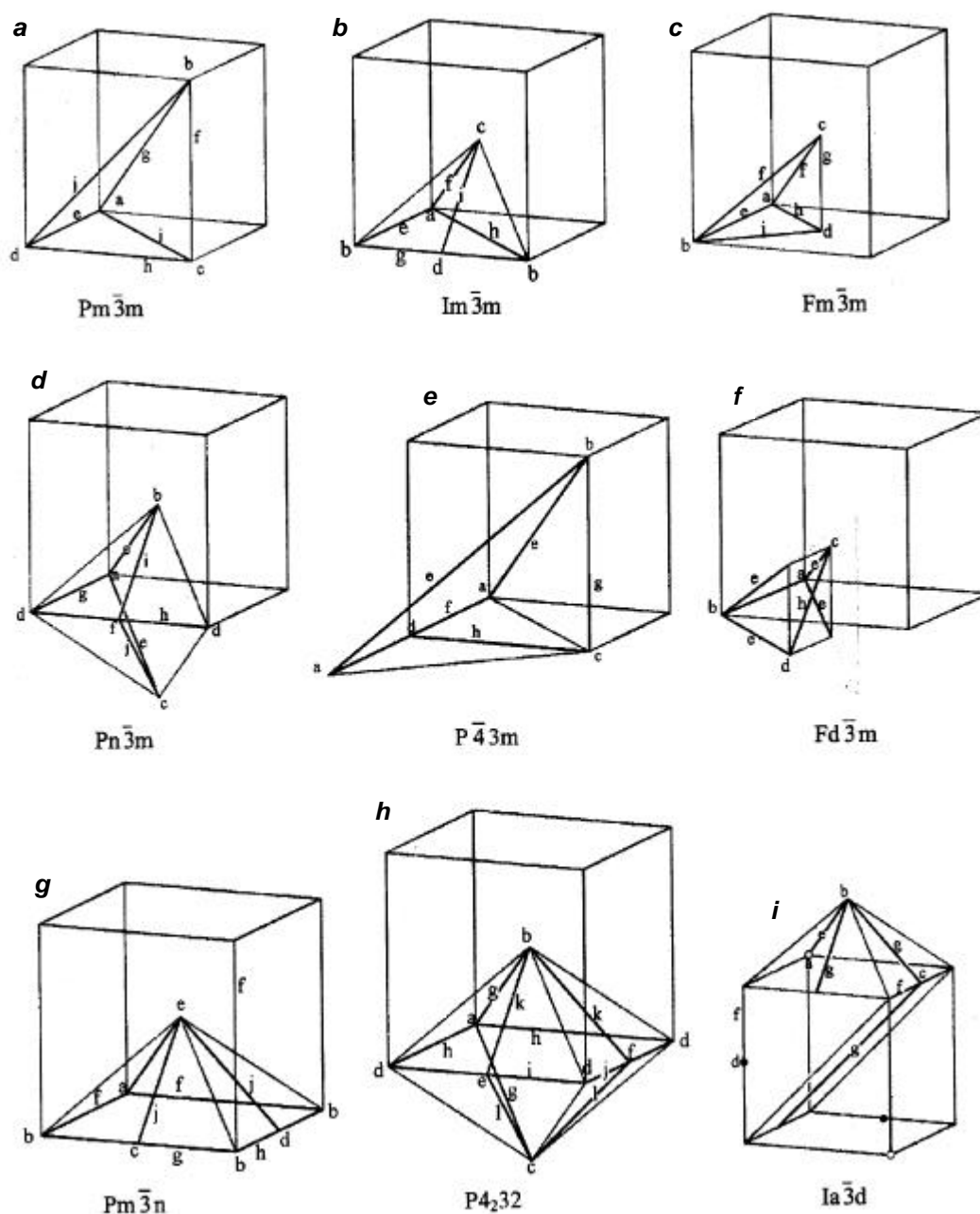


Figure 1. Asymmetric units for various cubic space groups. The bounding cube is $1/8$ of a cubic unit cell, except for $Ia\bar{3}d$, where the asymmetric unit is displayed in $1/64$ of a unit cell. Letters marking special points and line segments are the Wyckoff labels given in *The International Tables for Crystallography*. Asymmetric units displayed are the ones given in *The International Tables for Crystallography*, except for $Ia\bar{3}d$.

polygons interconnected by a branching catenoidal tunnel system and (3) the complete structure in the primitive cubic unit cell or a rhombic dodecahedron (for a face-centred cubic space group) or the 14-faced 'Thompson tetra-kaidecahedron', which can be repeated to fill all space for the body-centred cubic space groups.

We have asked ourselves the question: what possibilities exist if we ask for TPMBS with *cubic* symmetry generated by structural units that span *finite boundaries all of whose edges are straight lines* (diad axes)? In their 1996 paper, Fischer and Koch²⁰ completed their classification of minimal surfaces 'generated from skew polygons that are disc-like spanned, from catenoid-like surface patches, from branched catenoids, from multiple catenoids, or from infinite strips'. They went on to say: 'It may, however, be possible to find 3-periodic minimal surfaces without self-intersection which contain straight lines and are generated from surface patches other than those described . . .'. The present work is an exploration of these other possibilities. It can be regarded as a sequel to an earlier paper³² which described some new possibilities for TPMBS with *non-cubic* symmetries, and in which our method of approach based on 'asymmetric units' was set out in detail.

The P-family

The framework I of diad axes illustrated in Figure 4 results from applying the operations of the $m\bar{3}m$ at ver-

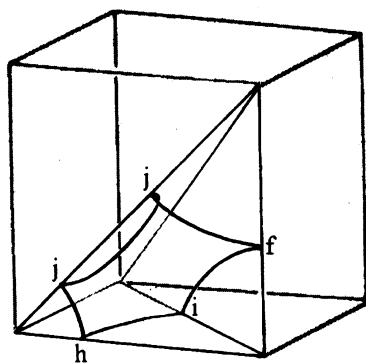


Figure 2. Fundamental patch for Schoen's OCTO.

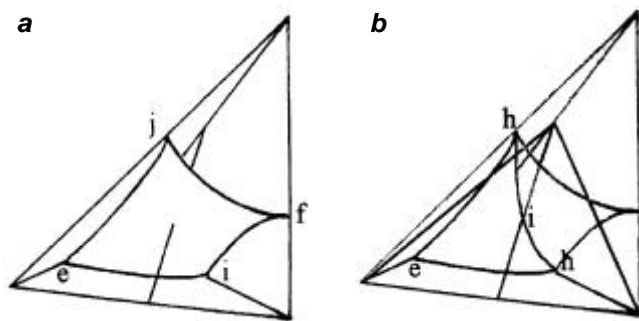


Figure 3. Fundamental patch for Schoen's IWP.

tex *a* of Figure 1 *b* to the diad segment *cd*. Notice that it consists of the diagonals of all the hexagonal faces of a *truncated octahedron*. Notice also that it has six octagonal circuits and twelve quadrilateral circuits. The framework II in Figure 4 is obtained similarly by applying the $4/mmm$ symmetry at a point *b*. It consists of two of the octagons and four of the quadrilaterals. When all the octagons and quadrilaterals are spanned by minimal surfaces, we get a pair of *saddle polyhedra*. (They are named by Pearce³³ 'the saddle cube dodecahedron' and 'the augmented universal hexahedron'). They fit together in a space-filling arrangement. If only the *quadrilaterals* are spanned, we get the P-surface $(Im\bar{3}m)cdh$. The quadrilateral patch is a *generating patch* consisting of four of the fundamental patches. If only the octagons are spanned, we get Neovius's C(P), $(Im\bar{3}m)cde$. The edge *cd* of the fundamental patch is a portion of a (free) diad axis embedded in the surface. It is expedient to indicate this important feature in the symbol string; we do this by capitalizing the Wyckoff letter associated with an embedded axis. That is, we write $(Im\bar{3}m)hI$ and $(Im\bar{3}m)eI$ for P and C(P), respectively. The skew octagon is a generating patch for C(P) (the Neovius surface); each octagonal patch consists of eight fundamental patches. More complicated configurations are possible. Framework I can be 'minimally spanned' by connecting all the quadrilaterals by tunnels with a junction around the centre of the figure. Since the centre is a Wyckoff position *a*, we call this surface *Pa*. Similarly, the C(P) octagons can be tunnelled to the centre. We can similarly connect either the four quadrilaterals of framework II by tunnels, or connect the two octagons by a 'catenoid-like' neck. The various names

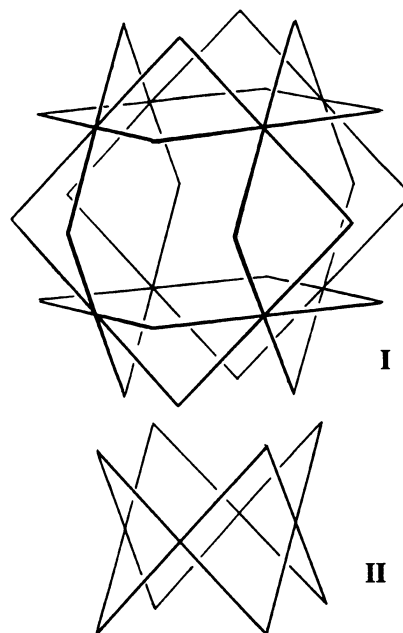


Figure 4. Diad frameworks for $Im\bar{3}m-Pm\bar{3}m$.

for these four TPMBS, together with the genetic specifications, are:

Pa ($\text{Im } \bar{3} \text{ m}$) efI ('Schoen's Batwing',³⁴)

Pb ($\text{Im } \bar{3} \text{ m}$) egI ('Schoen's C21(P)',³⁴)

C(P)a ($\text{Im } \bar{3} \text{ m}$) fhl (Gozdz and Holyst's 'Butterfly',²²
'Schoen's Manta',³⁴)

C(P)b ($\text{Im } \bar{3} \text{ m}$) ghI (Koch and Fischer's C(P)/H²⁰,
'Schoen's C15(P)',³⁴)

The same frameworks I and II shown in Figure 4 can be spanned in other ways, giving TPMBS with different G–H symmetries. The quadrilaterals of framework II can be connected *in pairs* by a catenoidal tunnel. We have named the resulting surface P2b. It is ($\text{Pm } \bar{3} \text{ n}$) $fhlJJ$, with symmetry $\text{Pm } \bar{3} \text{ n-Pm } \bar{3}$.

Framework I can be regarded as a structure built from four dodecagonal circuits – each dodecagon is a re-entrant polygon formed from three quadrilaterals with a common vertex. Linking these four 12-gons by a tetrahedral tunnel junction gives the surface P3a, ($\text{Pn } \bar{3} \text{ m}$) $ecgIJ$, with symmetry $\text{Pn } \bar{3} \text{ m-P } \bar{4} \text{ 3m}$.

The D-family

The two frameworks III and IV of Figure 5 are constructed from the diad axes of the space group $\text{Pn } \bar{3} \text{ m}$. Framework III can be seen as the set of diagonals of all the square faces and of four of the hexagonal faces of a truncated octahedron tetrahedrally disposed with the symmetry $\bar{4} \text{ 3m}$. Framework IV consists of two of the dodecagons and six of the quadrilaterals, and we again get a saddle polyhedron, here of symmetry $\bar{3} \text{ m}$, by spanning these circuits. The two saddle polyhedra together constitute a

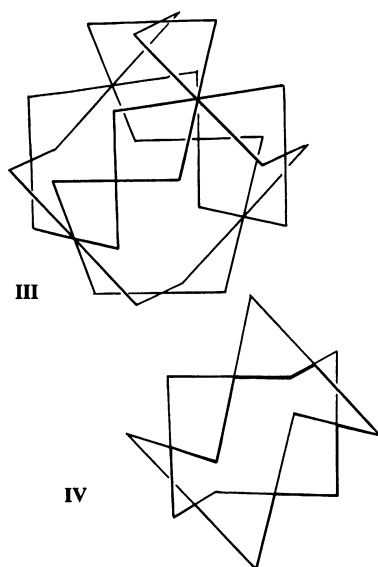


Figure 5. Diad frameworks for $\text{Pn } \bar{3} \text{ m-Fd } \bar{3} \text{ m}$.

space-filling pair. The quadrilaterals are generating patches for D ($\text{Pn } \bar{3} \text{ m}$) HI and the dodecagons are generating patches for C(D) ($\text{Pn } \bar{3} \text{ m}$) $ecHI$. Minimally spanning the frameworks III and IV in other ways gives rise to six more TPMS with the same symmetry $\text{Pn } \bar{3} \text{ m-Fd } \bar{3} \text{ m}$ as D and C(D):

Da ($\text{Pn } \bar{3} \text{ m}$) $ecgHI$

C(D)a ($\text{Pn } \bar{3} \text{ m}$) $ecgHI$ (Brakke's Starfish (ref. 34))

Dc ($\text{Pn } \bar{3} \text{ m}$) $ecHIje_c$

C(D)c ($\text{Pn } \bar{3} \text{ m}$) $HIjd$ (Koch and Fischer's C(D)/H²⁰)

D2a ($\text{Pn } \bar{3} \text{ m}$) $ecHI$

D3a ($\text{Pn } \bar{3} \text{ m}$) $ecHI$

A generating patch for C(D)a is a pair of C(D) dodecagons connected by a catenoidal tunnel. Observe that three D quadrilaterals of framework III share a common vertex. Four of these quadrilateral triples can also form an unconnected framework which we name III*. Two ways of spanning III* are D'a ($\text{Pn } \bar{3} \text{ m}$) $ecge_cHI$ and D3'a ($\text{Pn } \bar{3} \text{ m}$) $ecgIH$. However, experimentation with Evolver shows these configurations to be non-minimal.

The surface D2c has the symmetry $\text{P4}_2\text{32-F4}_1\text{32}$. It is obtained by connecting three pairs of D-quadrilaterals by a tunnel junction around the centre of framework IV. It is more easily visualized as a pair of C(D) dodecagons joined by tunnels at three of their common 90° vertices (Figure 6). It is ($\text{P4}_2\text{32}$) $dgJKKII$.

The F surface

Framework V shown in Figure 7 has eight skew hexagonal circuits. Each hexagon has six right angles and symmetry $\bar{3} \text{ m}$. It is the 'Petrie polygon' of a cube. It is a generating patch for the-D surface, consisting of 12 fundamental patches. Spanning all eight of the hexagons gives a space-filling saddle polyhedron (Pearce's 'bcc octahedron'). In the D-surface just four of the hexagons of Figure 7 are spanned, giving a configuration with symmetry $\bar{4} \text{ 3m}$.

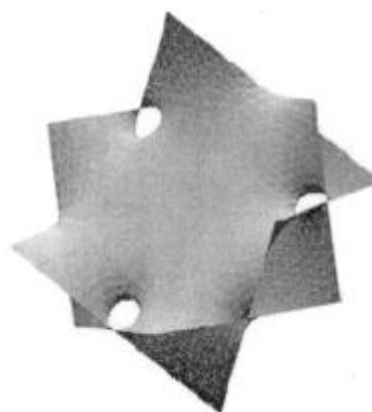


Figure 6. Generating unit for the surface D2c.

The centres of the four hexagonal films can be drawn together and joined by a tetrahedral tunnel system to give the surface $(F\bar{4}3m)egH$, which we shall name F, with symmetry $P\bar{4}3m-F\bar{4}3m$. It is the simplest member, after D itself, of the unnamed sequence displayed on Brakke's website.

P–D hybrids

Framework VI in Figure 8 is made up of the diad axes of $Fd\bar{3}m$. It can be understood as the set of diagonals of the hexagonal faces of a truncated tetrahedron (Friauf tetrahedron). It has six quadrilateral circuits and four hexagonal circuits. All angles of these skew quadrilaterals and skew hexagons are 60° . The skew quadrilateral is the Petrie polygon (PP) of a tetrahedron and the hexagon is the PP of an octahedron. Spanning all the circuits produces a space-filling polyhedron³³. The quadrilateral patch is a generating patch for D, consisting of eight fundamental patches. The hexagonal patch is a generating patch for P, consisting of 24 fundamental patches. Two new TPMS with symmetry $Fd\bar{3}m-F\bar{4}3m$ can be obtained by spanning the framework in alternative ways. Either the quadrilateral circuits or the hexagonal circuits can be joined by

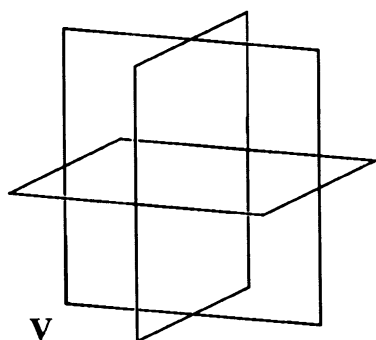


Figure 7. Diad framework for $P\bar{4}3m-F\bar{4}3m$.

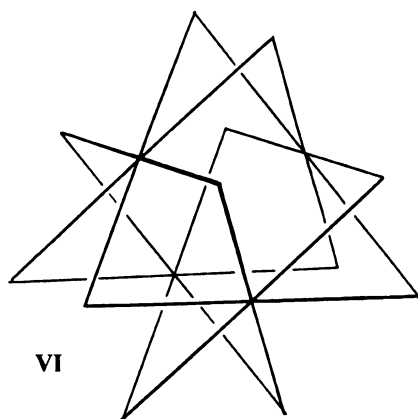


Figure 8. Diad framework for $Fd\bar{3}m-F\bar{4}3m$.

a tunnel junction around the centre of the framework, giving

$$DPa(Fd\bar{3}m)e_c e_b H$$

$$PDa(Fd\bar{3}m)efH$$

The Y family

The rather curious Figure 9 is formed from the diad axes of $I4_132$. The centre is at the point with point symmetry 32 . It has two nonagon circuits (the skew nonagon has three edge lengths, in the ratio of $1 : 3 : 2\sqrt{2}$ and the angles that are alternately 90° and 60°) and three hexagonal circuits. The labels on the vertices are coordinates referred to a unit cell of edge length eight centred at the 32 position b . The nonagon is a generating patch for Koch and Fischer's $C(Y)$, which in our system is described as $(I4_132)efH_c H_d$ (where H_c and H_d refer to the short and long segments ca and ad of the diad axes h) or, simply, $(I4_132)efHH$. The hexagon generates Y , $(I4_132)FHHg$, which turns out to be D in disguise³⁵. Connecting the two nonagon circuits by a catenoidal tunnel gives Fischer and Koch's $C(Y)/H^{20}$, which in our nomenclature would be called $C(Y)b$. We get one more new surface Yb (Figure 10) by connecting the three hexagons by a Y-shaped junction. The G/H symmetry of $C(Y)$, $C(Y)b$ and Yb is $I4_132-P4_332$.

S and G

The surface S is $(Ia\bar{3}d)aG_L G_S$. The subscripts L and S refer to the long and short portions – length ratio $3 : 1$ – of

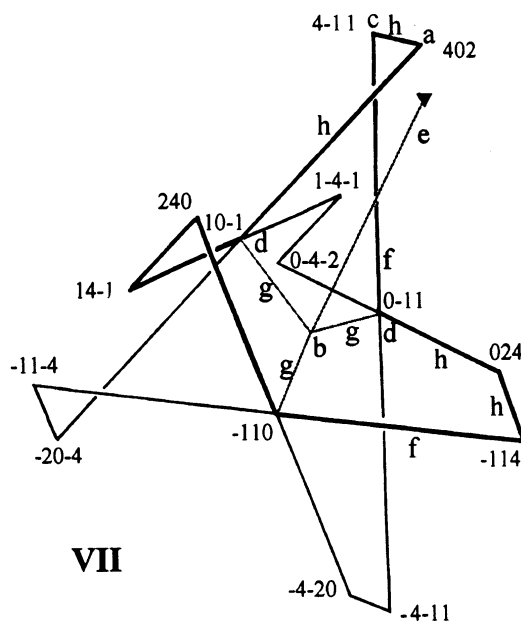


Figure 9. Diad framework for $I4_132-P4_332$.

the diad axes consisting of Wyckoff positions g . A dodecagonal generating patch for S is obtained by applying the $\bar{3}$ symmetry centred at a to the fundamental patch. $C(S)$, the ‘complement’ of S , $(Ia\bar{3}d)dG_LG_S$, with an octagonal generating patch, turns out to be P in disguise³⁵. Schoen’s gyroid G (Y^* in the nomenclature of Koch and Fischer) has no embedded diad axes at all; it is a balance surface by virtue of the inversion centres a and centres of $\bar{4}$ symmetry d , that lie on the surface. It is $(Ia\bar{3}d)adg$. The symmetries of S and G are, respectively, $Ia\bar{3}d-I4\bar{3}d$ and $Ia\bar{3}d-I4_132$. The nodal surface $C(Y^*)$ of von Schnering and Nesper also has $G-H$ symmetry $Ia\bar{3}d-I4_132$. A corresponding minimal surface may exist. We were unable to discover any other TPMS with $Ia\bar{3}d$ symmetry.

$\pm Y$ and $C(\pm Y)$

Finally, the surfaces $\pm Y$ and $C(\pm Y)$ span three non-intersecting families of diad axes and have the symmetry $Ia\bar{3}-$

$Pa\bar{3}$. There are no closed circuits of diad axes for this system but we mention it for, we hope, completeness²¹.

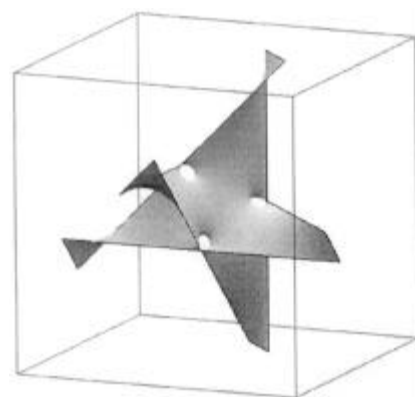


Figure 10. Generating unit for the surface Y_b .

Table 1. Nomenclature and data for cubic TPMS

Space groups G–H and diad frameworks	Surface name and references	Fundamental patch	Labyrinth s	Area per cubic unit cell of G	$-c$	Flat points and ‘special’ points	Order
$Im\bar{3}m-Pm\bar{3}m$						c, d	1, 0
I, II	(1) P Schwarz ¹¹	hI	E	2.345	4	$h(x, x, 0)$ 0.325	0
	(2) C(P) Neovius ¹²	eI	H	3.52564	16	$e(x, 0, 0)$ 0.410	2
I	(3) Pa ‘Schoen’s Batwing’ ³⁴	efI	H, bf	5.022	48	$f(x, x, x)$ 0.127 $e(x, 0, 0)$ 0.165	1 2
	(4) C(P)a Gozdz and Holyst’s BFY (Butterfly) ²² ; ‘Schoen’s Manta’ ³⁴	fhI	E, bf	4.964	36	$h(x, x, 0)$ 0.139 $f(x, x, x)$ 0.106	0 1
	(5) Pb ‘Schoen’s C21(P)’ ³⁴	egI	H, ag	3.678	40	$g(\frac{1}{2}, x, 0)$ 0.173 $e(x, 0, 0)$ 0.408	0 2
	(6) C(P)b Koch and Fischer’s C(P)/H ²⁰	ghI	E, ag	3.607	28	$g(\frac{1}{2}, x, 0)$ 0.023 $h(\frac{1}{2}, x, x)$ 0.16	0 0
$Pn\bar{3}m-P4\bar{3}m$ (bc)(ij)						b, f	1, 0
I	(7) P3a (new)	$ecgIJ$	ab_c, b_ae_c	4.629	32	$e(x, x, -x)$ 0.132 $g(x, 0, 0)$ 0.250	1 2
$Pm\bar{3}n-Pm\bar{3}$						c, d, e	0, 0, 1
II	(8) P2b (new)	$fhJJ$	bah	3.615	28	$f(\frac{1}{2}, \frac{1}{2}, x)$ 0.0612 $h(x, \frac{1}{2}, 0)$ 0.3395	2 0
$Pn\bar{3}m-Fd\bar{3}m$ (bc)(ij)						b, d, f	1, 0, 0
III, IV	(9) D Schwarz ¹¹	HI	E_c	1.920	4		
	(10) C(D) Schoen ¹³	$ecHI$	ac^I	3.9548	36	$e(x, x, -x)$ 0.200	4
III	(11) Da (new)	$ebecgHI$	ak, e_bk^Icg	4.817	92	$g(x, 0, 0)$ 0.407 $e(x, x, x)$ 0.168 $e(x, x, -x)$ 0.131	0 1 4
	(12) C(D)a Brakke’s Starfish ³¹ (ref. 34)	$ebgHI$	akg, ck^I, E_c	4.723	60	$g(x, 0, 0)$ 0.141 $e(x, x, x)$ 0.173	0 1

(Table 1. Contd.)

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(Table 1. Contd.)

Space groups G–H and diad frameworks	Surface name and references	Fundamental patch	Labyrinth s	Area per cubic unit cell of G	$-c$	Flat points and ‘special’ points	Order
IV	(13) D3a (new)	$e_c gHI$	ak, gck^l	3.877	60	$g(x, 0, 0)$ 0.205 $e(x, x, -x)$ 0.1024	0 1
	(14) D2a (new)	$e_b e_c HI$	$ak, ck^l e_b$	4.693	68	$e(x, x, x)$ 0.156 $e(x, x, -x)$ 0.110	1 4
	(15) Dc (new)	$e_j e_c HI$	akj, ck^l	4.10925	84	$j(\frac{1}{4} + x, \frac{1}{4}, x - \frac{1}{4})$ 0.19 $e(x, x, -x)$ 0.21	0 1
	(16) C(D)c Koch and Fischer’s C(D)/H ²⁰	$djHI$	E_c, ak, jk^l	4.109	52	$j(\frac{1}{4} + x, \frac{1}{4}, x - \frac{1}{4})$ 0.15	0
P4 ₂ 32-F4 ₁ 32 (bc)(kl), (ij)(ef)						b, d, e, f	1, 0, 0, 0
IV	(17) D2c (new)	$dg_c JKKII$	$al_f, cl_e a^K$	4.047	32	$g(x, x, x)$ 0.02 $l(\frac{1}{4}, \frac{1}{4} + x, x - \frac{1}{4})$ 0.2	1 0
P $\bar{4}$ 3m-F $\bar{4}$ 3m (ab)(cd)(e ₁ e ₂)(fg)						c, d	0, 0
V	(18) F Brakke ³⁴	$e_l gH$	E_2, ag	2.594	16	$e(x, x, x)$ 0.10 $g(\frac{1}{2}, \frac{1}{2}, x)$ 0.21	1 0
Fd $\bar{3}$ m-F $\bar{4}$ 3m (ab)(cd)						c, d	1, 1
VI	(19) DPa (new)	$e_{ac} e_{ab} H$	$F, e_{ac} b$	5.882	20	$e(x, x, x)$ 0.054 $e(x, x, -x)$ 0.066	1 1
	(20) PDa (new)	efH	$E_{ab}, e_{ac} b$	5.985	24	$e(x, x, x)$ 0.045 $f(x, 0, 0)$ 0.091	1 0
I4 ₁ 32-P4 ₃ 32 (ab)(cd)(gh)						a, c, d	1, 0, 0
VII	(21) C(Y) ¹⁴	$eFHH$	$bg_L e$	4.43	24	$e(x, x, x)$ 0.08	1
	(22) Yb (new)	$g_s e g_s FHH$	$ee^b g_L$	4.57	48	$g_s(-x, x, 0)$ 0.075 $e(x, x, x)$ 0.052	0 1
	(23) C(Y)b Koch and Fischer’s C(Y)/H ²⁰	$g_s g_L g_s FHH$	$bg_L g_s$	4.58	40	$g_s(-x, x, 0)$ 0.015 $g_L(x, -x, 0)$ 0.015	0 0
Ia3d-I $\bar{4}$ 3d						a, b	1, 1
VIII	(24) S (ref. 14)	aGG	bff^{cd}	5.44	20		

Column 1: The space group pair G–H, the permutation of Wyckoff letters that corresponds to an automorphism of the group G (and thus gives rise to alternative but equivalent notations for the fundamental patches), and the framework that is to be spanned by the generating unit of the surface. Koch and Fischer¹⁴ have given, for every G–H pair, a list of the Wyckoff positions that necessarily lie on any balance surface with that G–H symmetry. From the data it is not difficult to deduce that the frameworks I–VII, the non-connected III*, and the S-dodecagon VIII exhaust the possibilities for the boundaries of a generating unit.

Column 2: The commonly accepted nomenclature for previously known TPMBS and our proposed names for the new varieties, a numbering system for the 26 cases, and references.

Column 3: The boundaries of the fundamental patches.

Column 4: The labyrinth graphs. Upper-case letters denote edges and consecutive pairs of lower-case letters denote edges of the labyrinth graphs. Symbols are to be understood with reference to the labelling of the asymmetric units in Figure 1. A superscript indicates the action of a symmetry; for example, under (11) Da, k is a vertex lying on a mirror face of Figure 1 d – conveniently chosen to be $(3/8, 1/8, 1/8)$ – and k^l is its image under the action of the diad rotation about axis l .

Column 5: The area of the portion of the surface in a cubic unit cell of the group G.

Column 6: $-c$, where c is the Euler characteristic of the portion of the surface in a primitive unit cell of the group H. The *genus* of the surface is $g = 1 - c/2$.

Column 7: Positions of the flat points³⁶ and ‘special’ points. Special points are those where the surface cuts a diad axis.

Column 8: The order b of the flat points. $b = 0$ indicates a ‘special’ point.

Summary

Table 1 gives data for each of the surfaces we have discussed. We believe that the 24 surfaces listed here, together with the infinite sequences mentioned in the following section, are all possibilities for minimal TPMBS with cubic symmetry that can be generated from a finite unit whose boundary consists entirely of diad axes.

Higher genus sequences

Higher genus varieties of some of the surfaces we have described are possible. Some of the possibilities have

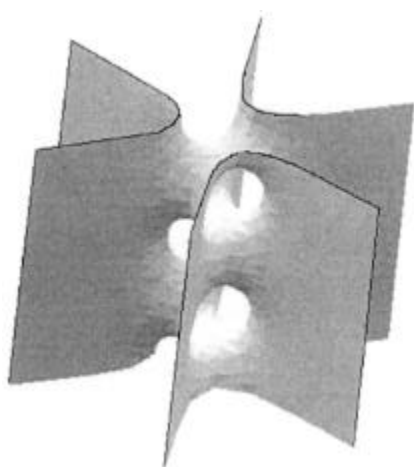


Figure 11. Non-self-intersecting configuration obtained from three planes through a line, by 'tunnelling'.

been explored by Schoen and Brakke and have been displayed on Brakke's website. They belong to sequences of surfaces, with increasing genus, that appear to converge in the limit to self-intersecting surfaces which may have embedded axes of 3-fold or 4-fold rotational symmetry, as well as embedded diads. Consider the self-intersecting surfaces $(\text{Im } \bar{3}m)EFIG$. Non-intersecting balance surfaces can be obtained by replacing the lines of self-intersection by rows of tunnels, as in Figure 11. In this way, we get the non-intersecting surfaces $(\text{Im } \bar{3}m)e^p f^q I g^r$. $(\text{Im } \bar{3}m)ef^q I$ is the 'Batwing' sequence and $(\text{Im } \bar{3}m)g^r eI$ are 'Schoen's C(P) surfaces'. We shall simply list, without further comment, all such sequences of cubic balance surfaces for which the existence of minimal surfaces with the suggested symmetry and topology seems plausible along with $-c$, where c is the Euler characteristic (Table 2). For reasons of space, we omit our criterion of 'plausibility'. We make no claim that minimal surfaces exist in all cases! However, it seems likely that Tables 1 and 2 contain all possible TPMBS with cubic symmetry that can be generated by units bounded only by straight edges.

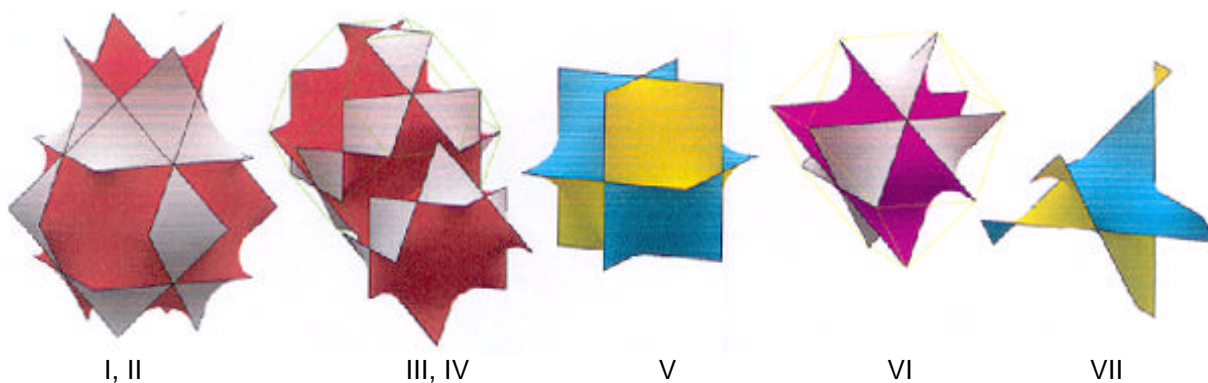
A gallery of minimal surfaces

'A gallery of minimal surfaces', consisting of six colour plates, presents illustrations of the generating units and unit cells for a selection of surfaces referred to in the text. These graphic representations were produced using Brakke's 'Surface Evolver'.

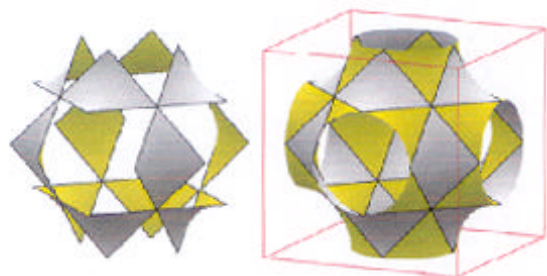
Table 2. Families of non-intersecting balance surfaces with cubic symmetry

$\text{Im } \bar{3}m\text{-Pm } \bar{3}m$			
I	$e^p f^q I$	$4(-5 + 9p + 8q)$	$p = 1$: Batwings
	$e^p h^q I$	$4(1 + 9p + 8q)$	
	$f^p h^q I$	$4(-5 + 8p + 6q)$	$q = 1$: Mantas
	$f^p e h^q I$	$8(2 + 4p + 3q)$	
II	$g^p h^q I$	$4(-5 + 6p + 6q)$	$q = 1$: Schoen's C(P) surfaces
	$g^p e^q I$	$4(-5 + 6p + 9q)$	$q = 1$: Schoen's C(P) surfaces
$\text{Pn } \bar{3}m\text{-P } \bar{4}3m$			
I	$e_c^p e_b^q IJ$	$4(1 + 4p + 4q)$	
	$e_c^p g e_b^q IJ$	$16(1 + p + q)$	
$\text{Pm } \bar{3}n\text{-Pm } \bar{3}$			
II	$g^p h^q JJ$	$4(1 + 3p + 3q)$	
	$g^p f h^q JJ$	$4(4 + 3p + 3q)$	
$\text{Pn } \bar{3}m\text{-Fd } \bar{3}m$			
III	$e_b^p g^q HI$	$4(1 + 8p + 6q)$	Brakke's Starfish
	$e_b^p e_c g^q HI$	$4(9 + 8p + 6q)$	
III*	$e_b^p e_c^q HI$	$8(1 + 4p + 4q)$	
	$e_b^p g e_c^q HI$	$32(4 + p + q)$	
$\text{P } \bar{4}3m\text{-F } \bar{4}3m$			
V	$e^p g^q H$	$4(-3 + 4p + 3q)$	$p = 1$: Brakke's unnamed sequence

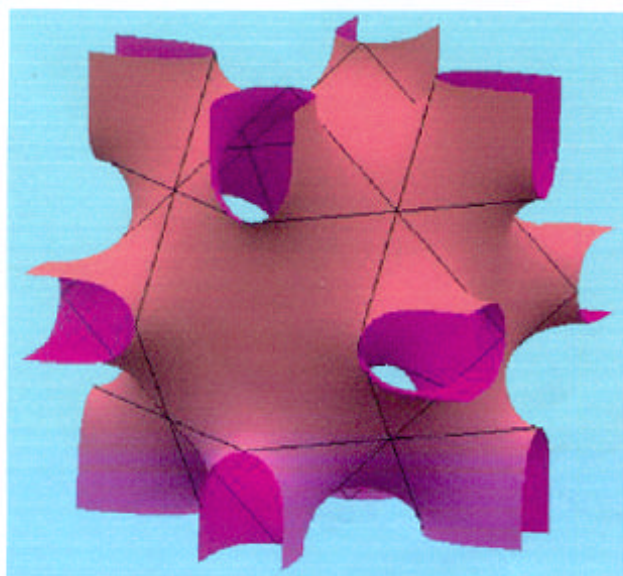
A gallery of minimal surfaces



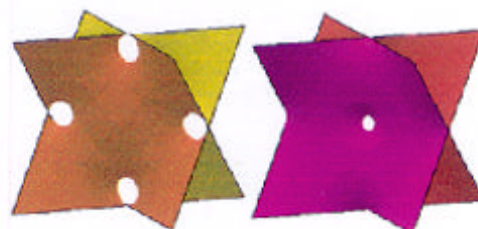
The space filling saddle polyhedra obtained by minimally spanning the frameworks I to VII.



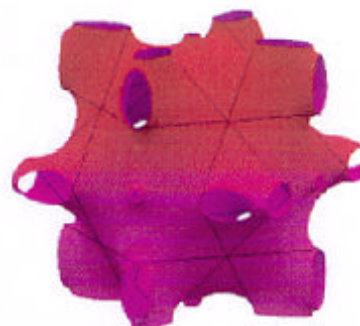
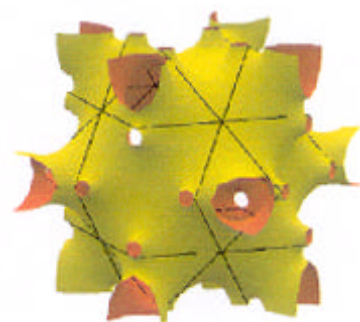
The twelve generating patches of **P** spanning circuits of framework I, and the extension of the configuration to a unit cell.

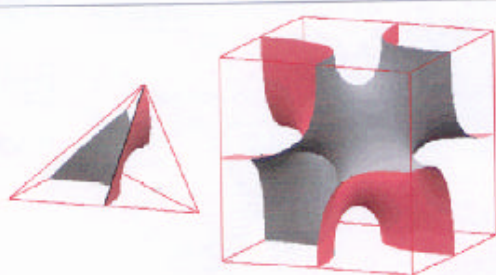


Neovius' surface **C(P)**

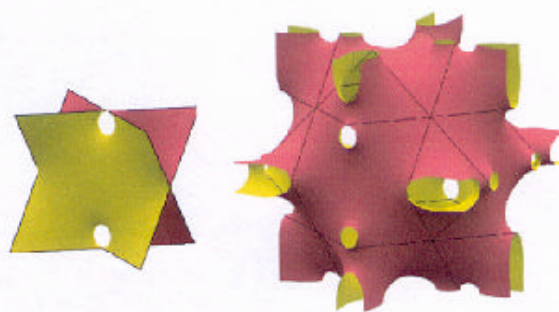
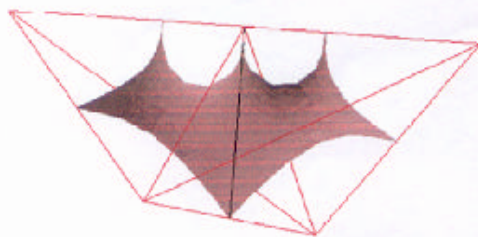
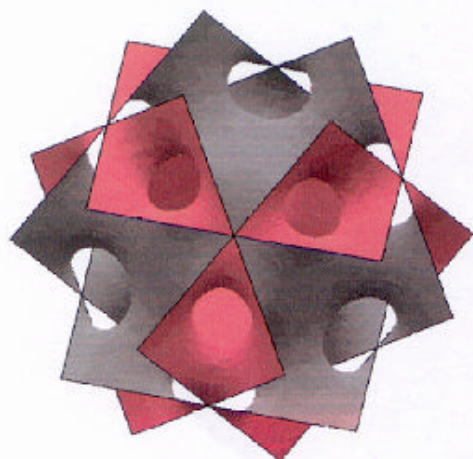
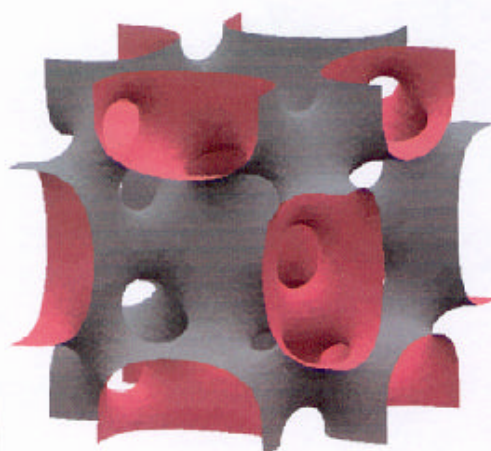


The generating units for **Pb** and **C(P)b** and below, the unit cells for **Pb** and **C(P)b**.

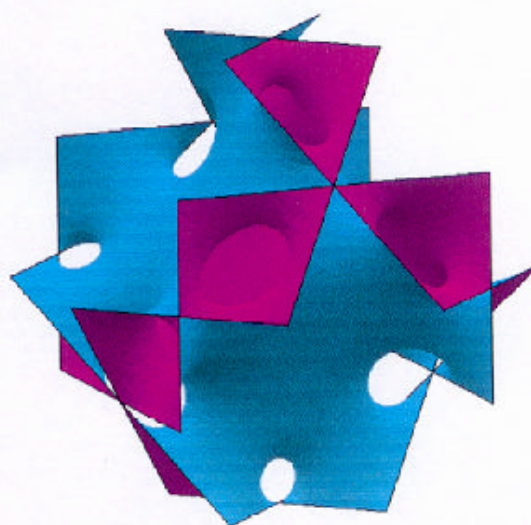




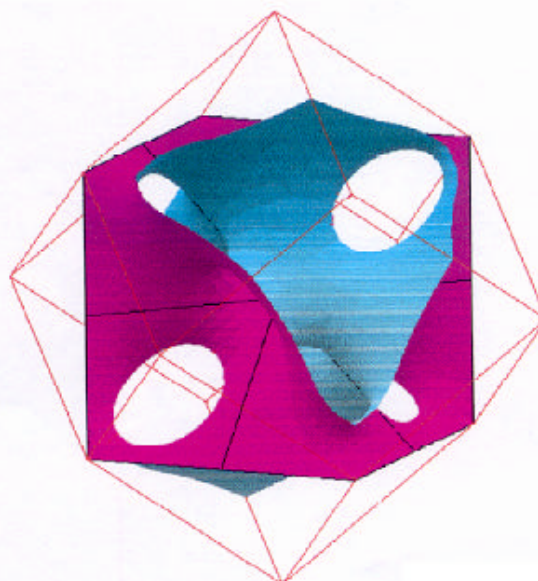
Fundamental patch of **Pa**, and 1/8 unit cell. Below: A cubic unit cell of **Pa**, and the generating unit (framework I minimally spanned), viewed along a threefold axis, and a pair of fundamental patches indicating the reason for the name 'batwing'.

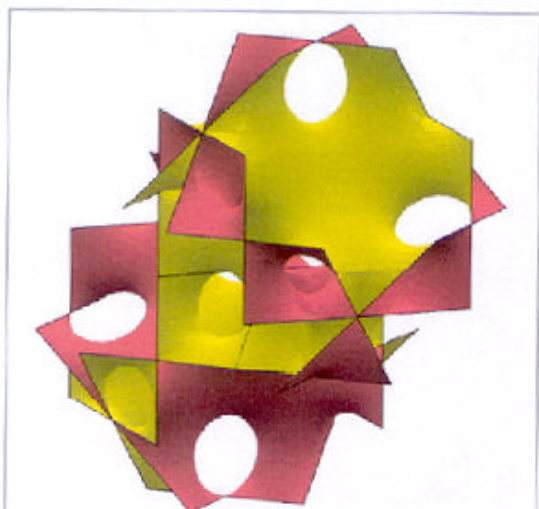


The generating patch and the unit cell of **Pb**

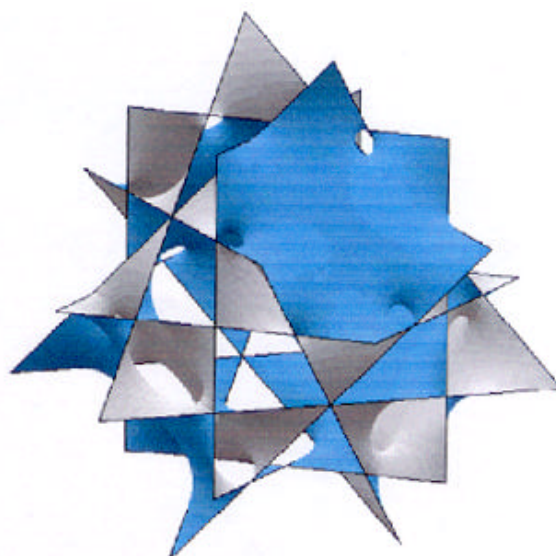


The generating unit for **Da** and below, the portion of the surface inside a rhombic dodecahedron six of whose faces are mirror planes, and six contain diads.

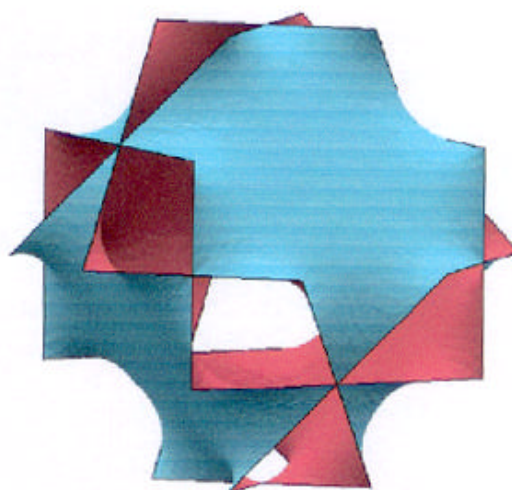
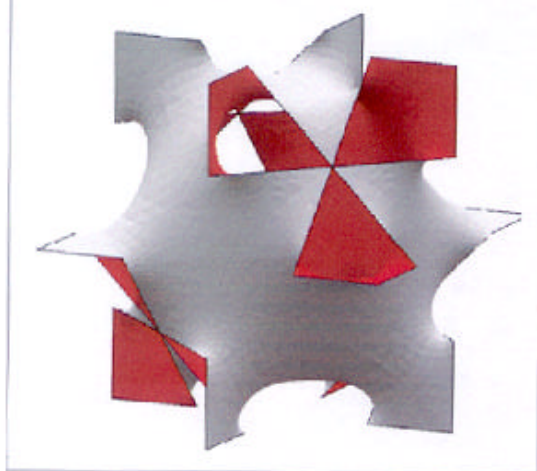




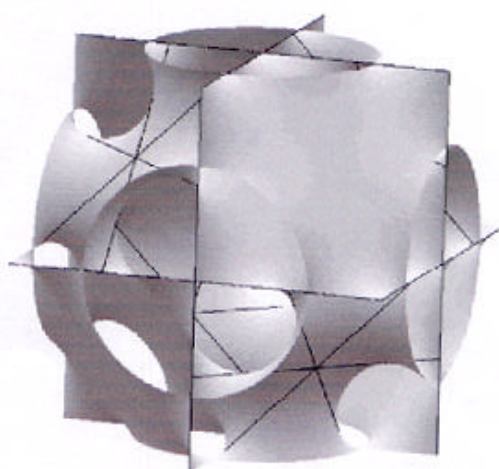
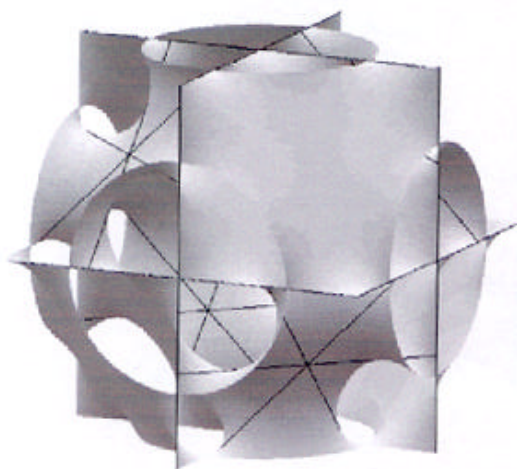
A pair of generating units for **D3a** and below, the **non-minimal** balance surface **D3'a** (obtained by using Surface Evolver to minimize the squared integrated mean curvature).



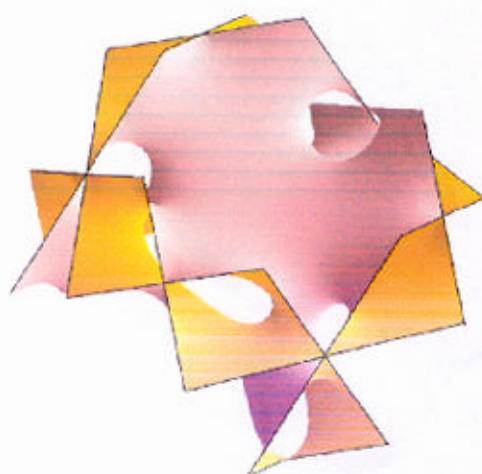
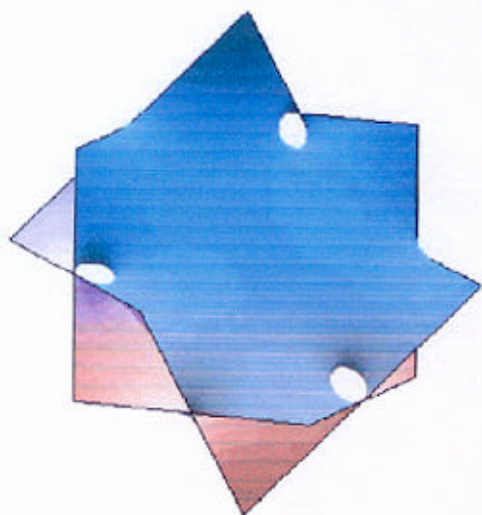
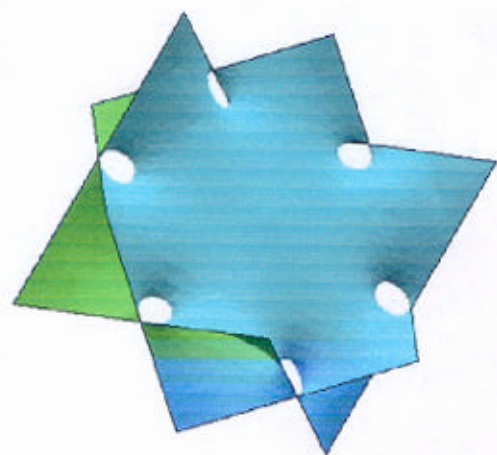
Portion of **D2c** consisting of four generating units



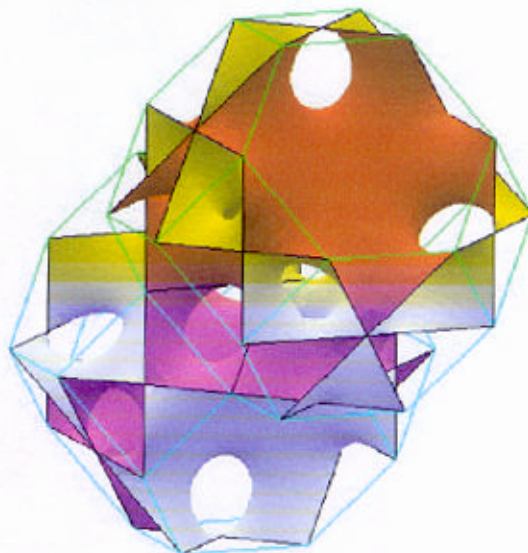
Four dodecagonal patches of Schoen's **C(D)**



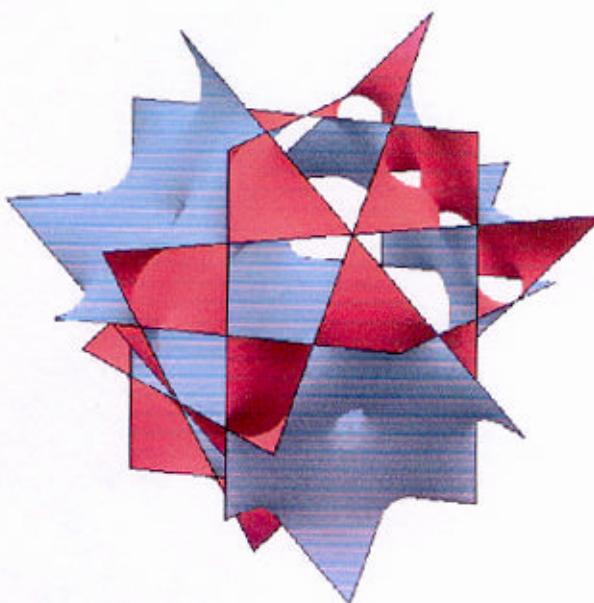
A stereo pair of images of the unit cell of Schoen's **C(D)**.



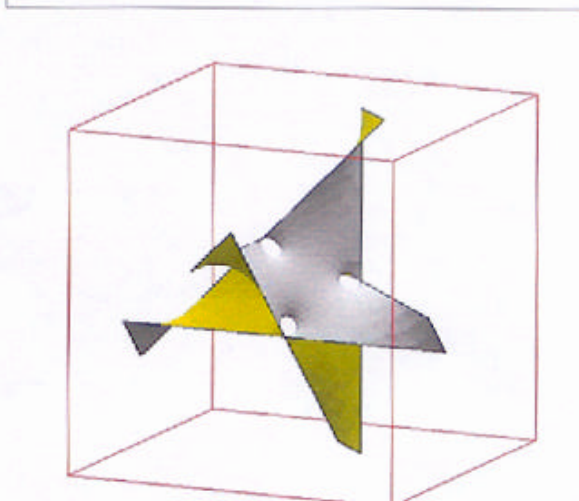
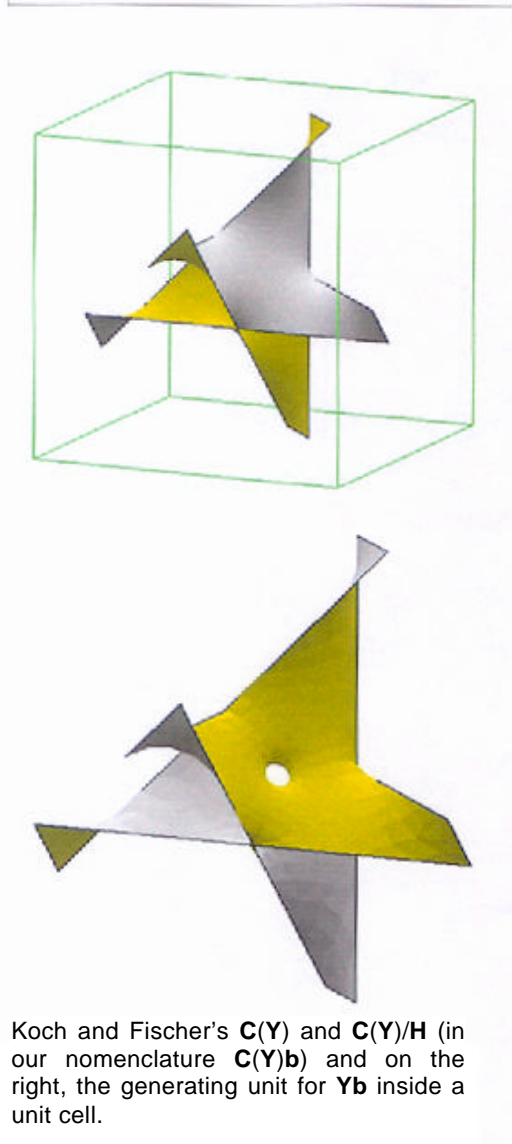
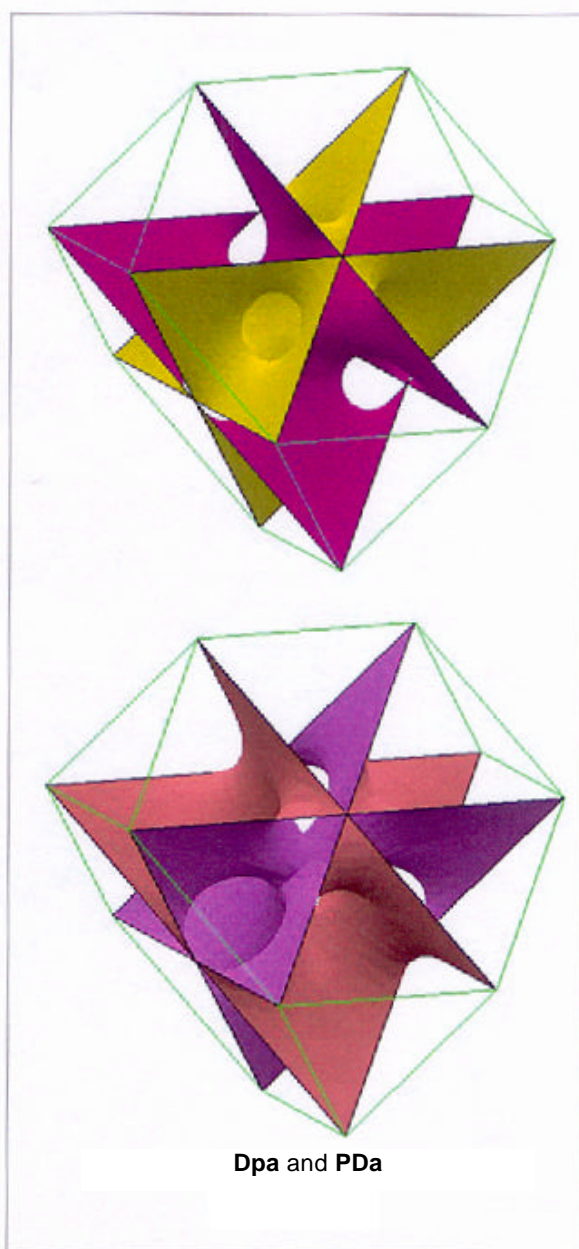
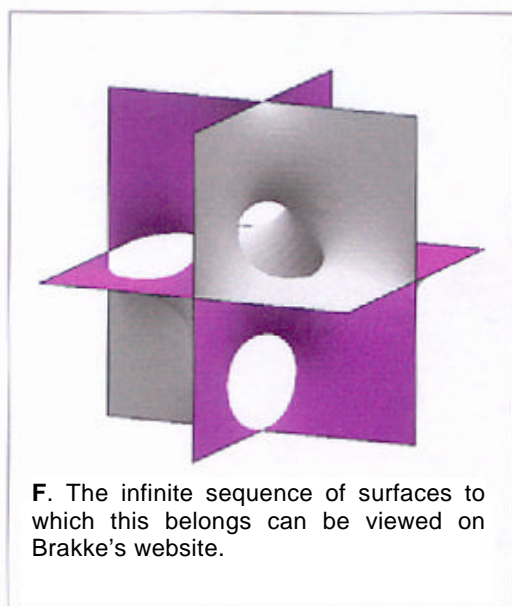
Generating units for **D_c**, **D_{2c}** and **D_{2a}**



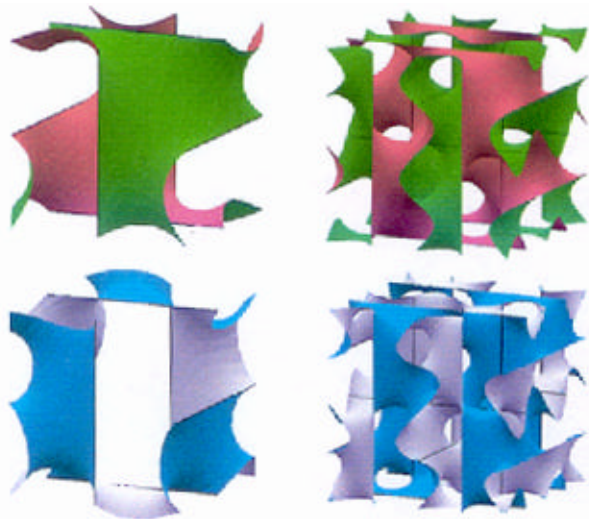
Two generating units for **D_{3a}**. Observe the space filling truncated octahedral building blocks, related by diad rotations about their face diagonals.



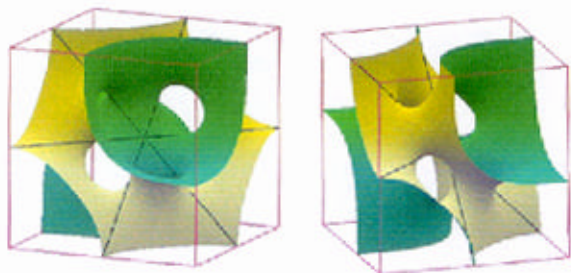
Four generating units of **C(D)_c**



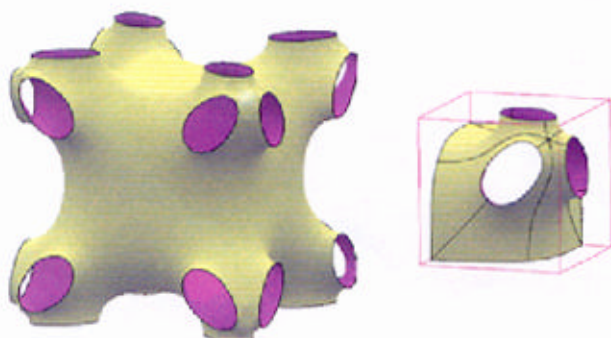
Below we illustrate a few examples of cubic minimal surfaces whose generating units are *not* bounded entirely by straight edges.



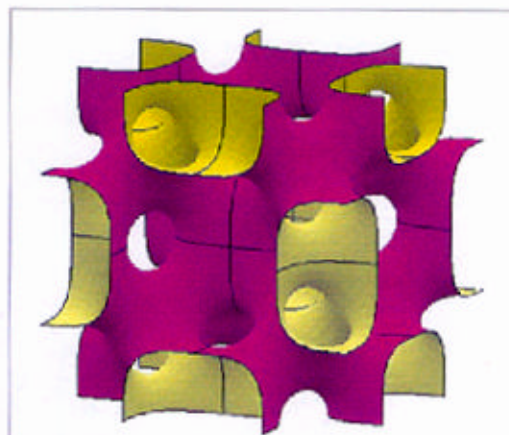
Koch and Fischer's $C(\pm Y)$ can be generated by a pair of nonagons each with three straight edges. This corresponds to $1/8$ of a unit cell and is illustrated, along with the unit cell. Below for $\pm Y$, two nonagons are linked by a tunnel.



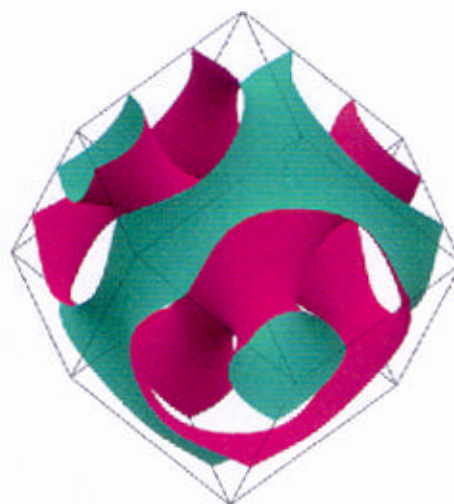
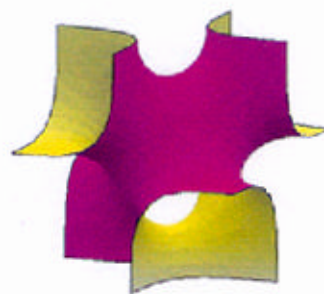
$1/8$ unit cell of a minimal balance surface with the same symmetry as P and $C(P)$. The patch shown has the same topology of Costa's (non-periodic) minimal surface.



A new non-balanced minimal surface generated by reflections: unit cell, and $1/8$ unit cell containing six fundamental patches. There exists a wide variety of non-balanced TPMS. Their classification remains an unexplored problem.



A non-balanced surface: A unit cell of Schoen's **FRD**. Generated by reflections in the faces of $1/8$ of the unit cell, which contains a patch with tetrahedral symmetry:



A 'double diamond' surface. A pair of surface of constant mean curvature belonging to the family of surfaces to which D (zero mean curvature) belongs. The triply periodic structure is generated by reflections in the faces of the rhombic dodecahedron.

1. Hyde, S., Andersson, S., Larsson, K., Blum, Z., Landh, T., Lidin, S. and Ninham, B. W., *The Language of Shape*, Elsevier, Amsterdam, 1997.
2. Plato, *Timaeus* (transl. Lee, H. D. P.), Penguin, Harmondsworth, 1965.
3. Kenner, H., *Bucky: A Guided Tour of Buckminster Fuller*, William Morrow, New York, 1973.
4. *The International Tables for Crystallography* (ed. Hahn, Th.), Kluwer Academic Publishers, Dordrecht, 1989. Essential data on the space groups can be found from a compact disc obtainable from the School of Crystallography, Birkbeck College, University of London, vol. A.
5. Bashkurov, N. M., A generalization of Fedorov's stereohedra method. *Sov. Phys. Crystallogr.* (transl.), 1959, **4**, 442–447.
6. Thompson, D'A. W., *On Growth and Form*, Cambridge University Press, 1917.
7. Andersson, S. and Hyde S. T., The intrinsic curvature of solids. *Z. Kristallogr.*, 1984, **168**, 1–17.
8. Klinowski, J., Mackay, A. L. and Terrones, H., Curved surfaces in chemical structure. *Philos. Trans. R. Soc. London*, 1996, **354**, 1969–2192.
9. Mackay, A. L., Flexi-crystallography: curved surfaces in chemical structures. *Curr. Sci.*, 1995, **69**, 151–160.
10. Coxeter, H. S. M., Regular skew polyhedra in three and four dimensions and their topological analogues. *Proc. Lond. Math. Soc.*, 1937, **43**, 33–62.
11. Schwarz, H., Über Minimalflächen. *Monatsber. Berlin Akad.*, April 1865; *Gesammelte Mathematische Abhandlungen*, Springer, Berlin, 1890, vol. 1.
12. Neovius, E. R., *Bestimmung zweier speciellen Minimalflächen*, Akad. Abhandlungen, Helsingfors, 1883.
13. Schoen, A. H., Infinite periodic minimal surfaces without self-intersections. NASA Technical Report TN D-5541, Washington DC, 1970.
14. Koch, E. and Fischer, W., On 3-periodic minimal surfaces. *Z. Kristallogr.*, 1987, **179**, 31–52.
15. Fisher, W. and Koch, E., On 3-periodic surfaces with non-cubic symmetry. *Z. Kristallogr.*, 1988, **183**, 129–152.
16. Fischer, W. and Koch, E., New surface patches for minimal balance surfaces. I. Branched catenoids. *Acta Crystallogr.*, 1989, **A45**, 166–169.
17. Koch, E. and Fischer, W., New surface patches for minimal balance surfaces. II. Multiple catenoids. *Acta Crystallogr.*, 1989, **A45**, 169–174.
18. Fischer, W. and Koch, E., New surface patches for minimal balance surfaces. III. Infinite strips. *Acta Crystallogr.*, 1989, **A45**, 485–490.
19. Koch, E. and Fischer, W., New surface patches for minimal balance surfaces. IV. Catenoids with spout-like attachments. *Acta Crystallogr.*, 1990, **A45**, 558–563.
20. Fischer, W. and Koch, E., Spanning minimal surfaces. *Philos. Trans. R. Soc. London*, 1996, **A354**, 2105–2142.
21. Fischer, W. and Koch, E., Genera of minimal balance surfaces. *Acta Crystallogr.*, 1989, **A45**, 726–732.
22. Gozdz, W. and Holyst, R., From the Plateau problem to periodic minimal surfaces in lipids and diblock copolymers. *Macromol. Theory Simul.*, 1996, **5**, 321–332.
23. Karcher, H. and Polthier, K., Construction of triply periodic minimal surfaces. *Philos. Trans. R. Soc. London*, 1996, **A354**, 2077–2104.
24. Friedrichs, O. D., Dress, A. W. M., Huson, D. H., Klinowski, J. and Mackay, A. L., Systematic enumeration of crystalline networks. *Nature*, 1999, **400**, 644–647.
25. Weierstrass, K., Untersuchungen über die Flächen, deren mittlere Krümmung überall gleich Null ist. *Monatsber. Berlin Akad.*, 1866, 612–625.
26. Nitsche, J., *Lectures on Minimal Surfaces*, Cambridge University Press, 1989.
27. Fogden, A. and Hyde, S. T., Parametrization of triply periodic minimal surfaces. I. Mathematical basis of the construction algorithm for the regular class. *Acta Crystallogr.*, 1992, **A48**, 442–451.
28. Fogden, A. and Hyde, S. T., Parametrization of triply periodic minimal surfaces. II. Regular class solutions. *Acta Crystallogr.*, 1992, **A48**, 575–591.
29. Fogden, A. and Hyde, S. T., Parametrization of triply periodic minimal surfaces. III. General algorithm and specific examples for the irregular class. *Acta Crystallogr.*, 1993, **A49**, 409–421.
30. Brakke, K. A., The Surface Evolver. *Exp. Math.*, 1992, **1**, 141–165.
31. von Schnering, H. G. and Nesper, R., Nodal surfaces of Fourier series: fundamental invariants of structured matter. *Z. Phys. B*, 1991, **83**, 407–412.
32. Lord, E. A., Triply periodic balance surfaces. *Colloids Surf. A*, 1997, **129–130**, 279–295.
33. Pearce, P., *Structure in Nature is a Strategy for Design*, MIT Press, Cambridge Mass., 1978.
34. Brakke, K., www.susqu.edu/facstaff/b/brakke/
35. Koch, E. and Fischer, W., Triply periodic minimal balance surfaces: a correction. *Acta Crystallogr.*, 1993, **A49**, 209–210.
36. Koch, E. and Fischer, W., Flat points of minimal balance surfaces. *Acta Crystallogr.*, 1990, **A46**, 33–40.

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