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# New Surface Patches for Minimal Balance Surfaces. IV. Catenoids with Spout-Like Attachments

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## Abstract

The way in which Schoen [*Infinite Periodic Minimal Surfaces Without Self-intersections* (1970), NASA Tech. Note No. D-5541] derived a simply connected surface patch for a $C(H)$ surface cannot be generalized. One may, however, subdivide a $C(H)$ surface into larger patches that are not simply connected. Surface patches of analogous shape give rise to five families of minimal balance surfaces unknown so far: tetragonally and orthorhombically distorted $C(P)$ surfaces, surfaces complementary to Schoen's $R2$ and $R3$ surfaces with genus 25 and 37, respectively, and orthorhombic surfaces of a fifth family with genus 5 that are also complementary to $oP$ surfaces.


## 1. Schoen's $C(H)$ surfaces

Schoen (1970) described a family of minimal balance surfaces $C(H)$ complementary to the $H$ surfaces of Schwarz (1890). He derived a surface patch of a $C(H)$ surface by deformation of a suitably chosen surface patch of a $C(P)$ surface (Neovius, 1883). For this he started with a cube formed by six mirror planes. It delimits a disc-like patch of a $C(P)$ surface that is bounded by 12 plane lines of curvature, two of them on each face of the cube. The point group of such a surface patch is $.\bar{3}m$. The threefold rotation axis runs perpendicular to the surface patch, each of the three twofold axes bisects two opposite edges, and each of the three mirror planes contains two of the further six edges of the cube.

According to Schoen (1970) one may construct an analogous surface patch within a prism with a rhombus as cross-sectional view (rhombus angles of 60, 120°). The faces of such a prism also may be formed by mirror planes giving rise to hexagonal symmetry. The point group of the resulting surface patch (Fig. 1) is reduced to $2/m$ compared with that of a $C(P)$ surface. The twofold axis runs through the midpoints of the two 60° edges of the prism, while the mirror plane contains the two 120° edges. Such a surface patch may be extended by reflection at the prism faces. The resulting minimal balance surface was designated $C(H)$ by Schoen (1970) because it shows the same inherent symmetry $P6_3/mmc$-$P\bar{6}m2$ and, therefore, the same linear skeletal net as an $H$ surface. The genus of a $C(H)$ surface is 7.

Schoen's derivation emphasizes the mirror planes and the plane lines of curvature of a $C(H)$ surface. On the other hand, it is possible to choose larger surface patches which stress the twofold axes and the linear skeletal net. Such a view of the $C(H)$ surfaces is more similar to that used in previous papers of the present authors (Fischer & Koch, 1987, 1989*a*, *b*; Koch & Fischer, 1988, 1989).

The common linear skeletal net of an $H$ and a $C(H)$ surface disintegrates into plane nets of equilateral triangles stacked directly upon each other. Referred to the $H$ surface two kinds of triangle pairs are formed within these triangular nets, namely those which are generating circuits for catenoid-like surface patches and those which are not (*cf.* Koch & Fischer, 1988). Pairs of the latter kind may be related to more complicated surface patches of the $H$ surface which are, therefore, less useful than the catenoids. Such a more complicated surface patch consists of three disc-like fragments without common boundaries. Each fragment corresponds to the third part of a catenoid and has four boundary lines: two triangle edges and two plane lines of curvature connecting the triangle vertices. Each two of these fragments share two triangle vertices.

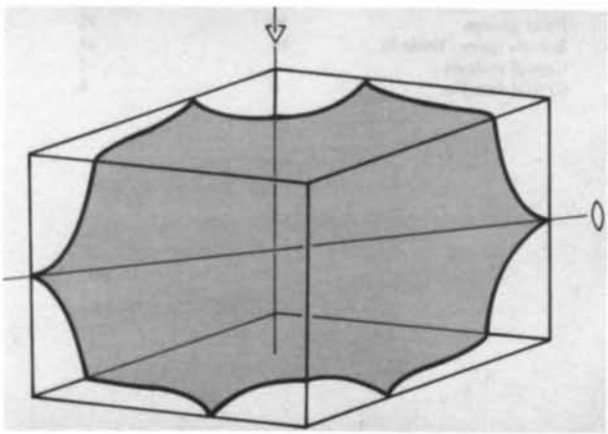

Fig. 1. Disc-like surface patch of a $C(H)$ surface as described by Schoen (1970).

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Both kinds of surface patches are delimited by space-filling hexagonal prisms. Six vertices of such a prism correspond to the vertices of the triangle pair under consideration, and the prism axis runs through the triangle centres. The rectangular prism faces are formed by mirror planes of the surface. A surface patch may be continued either by the reflections corresponding to the prism faces or by the twofold rotations that refer to the triangle edges. The reflections, however, are not necessary to generate the complete surface. Although both kinds of hexagonal prisms give rise to a space tiling the prisms share only entire rectangular faces whereas each hexagonal face is in contact with three hexagonal faces of other prisms.

Similarly, a $C(H)$ surface may be subdivided into two kinds of surface patches that are larger than those described by Schoen (1970):

(1) The catenoid-like surface patches of an $H$ surface correspond to catenoids with three spout-like attachments. The point group $\bar{6}m2$ of such a surface patch is the same as for the catenoids. The central lines of the spouts have site symmetry $mm2$ and run through the midpoints between two opposite triangle edges. Fig. 2 shows the lower half of such a surface patch. The entire patch has 12 boundary lines: the two triangles in the hexagonal prism faces and six plane lines of curvature within the six rectangular prism faces. Spouts of three neighbouring catenoids are united to three-armed handles. The central axes of these handles coincide with those prism edges that do not run through triangle vertices. Consequently, each catenoid is connected to six neighbouring catenoids *via* three of these three-armed handles.

(2) The other triangle pairs within a $C(H)$ surface belong to surface patches, the inner parts of which resemble catenoids with three ends. The corresponding point group is also $\bar{6}m2$, and the three ends point to the midpoints between opposite triangle edges, too. The symmetry in these directions is $mm2$. Fig. 3 represents the lower half of such a surface patch. The

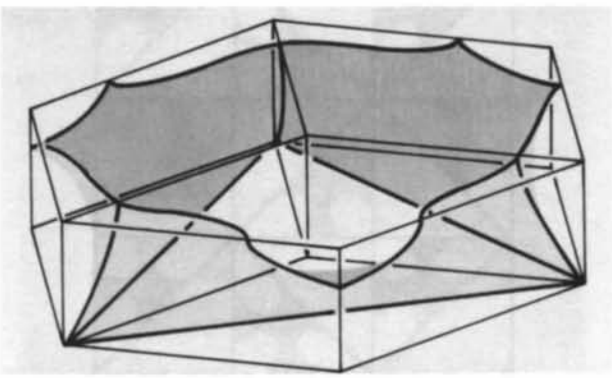


Fig. 2. Lower half of a catenoid with three spout-like attachments, *i.e.* of a $C(H)$ surface patch.

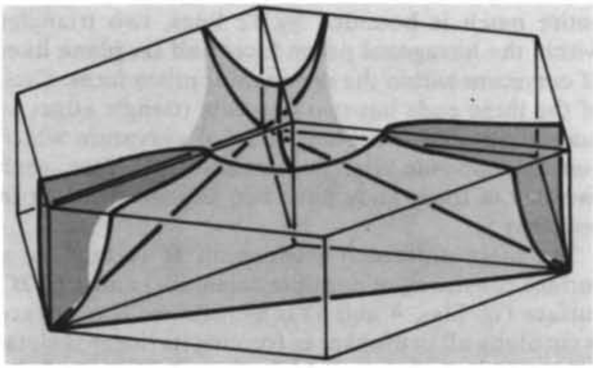
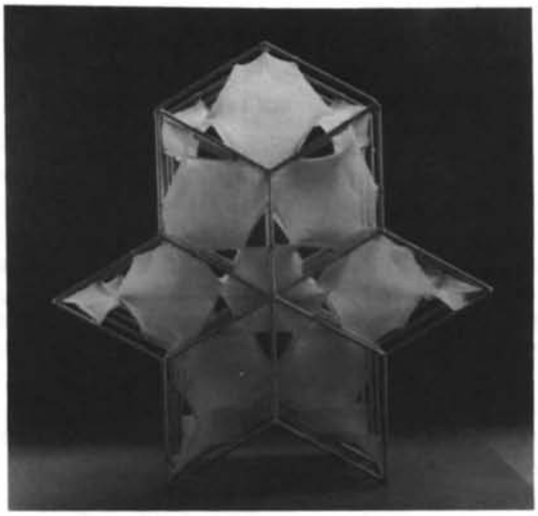


Fig. 3. Lower half of a catenoid with three ends, *i.e.* of a $C(H)$ surface patch.



(*a*)

(*b*)

Fig. 4. Model of a $C(H)$ surface: (*a*) viewed along **c**, (*b*) oblique view.

entire patch is bounded by 12 lines, two triangles within the hexagonal prism faces and six plane lines of curvature within the rectangular prism faces. Each of the three ends has two opposite triangle edges as boundaries and two plane lines of curvature which connect opposite triangle vertices. Therefore, each two of the three ends have two triangle vertices in common.

The main difference between an *H* surface (or a surface consisting of multiple catenoids) and a *C*(*H*) surface (*cf.* Figs. 4 and 5) is as follows: If a surface is cut along all twofold axes forming its linear skeletal net, an *H* surface (or an *MC* surface) falls into finite pieces, the catenoids (or the multiple catenoids). In contrast to this, a *C*(*H*) surface decomposes into two-dimensional infinite pieces with layer-group symmetry and bounded by two triangular nets of twofold axes.

## 2. Minimal balance surfaces *C*(*R*2)

The inherent symmetry of Schoen's (1970) *R*2 surface is *I*4/*mcm*-*P*4/*mbm*. The linear skeletal net disintegrates into an infinite set of parallel plane triangular nets (angles: 45, 45, 90°) stacked directly upon each other. As described for *H* surfaces the linear skeletal net of an *R*2 surface contains two kinds of triangle pairs that correspond to two different kinds of surface patches: catenoids bounded by two triangles and surface patches consisting of three disc-like fragments. In contrast to *H* surfaces these fragments have two triangle edges as boundary lines and two other lines, one or both of which are not plane lines of curvature because of the absence of corresponding mirror planes in the symmetry of *R*2 surfaces. The three fragments share the vertices of the triangles. The further lines connect neighbouring vertices of the triangles and may partly be chosen with some arbitrariness, *e.g.* as geodesics, but the point symmetry *m*.*m*2 of *R*2 surface patches has to be obeyed. Therefore, two fragments with symmetry *m*.. have to be congruent, whereas the third one must show symmetry *m*.*m*2.

As described above for *C*(*H*) surface patches one can derive surface patches for a new family of minimal balance surfaces from those of *R*2 surfaces.

The *R*2 catenoids correspond to catenoids with three spout-like attachments and point symmetry *m*.*m*2. In contrast to *C*(*H*) surfaces these spouts can only partly be bounded by plane lines of curvature. Again three spouts are united to three-armed handles, but each catenoid is connected only to five other catenoids by three of these handles. Two catenoids sharing the 90° vertices of their triangle pairs are connected twice.

The second kind of surface patches of an *R*2 surface refers to catenoids with three ends and symmetry *m*.*m*2. Each end is bounded by two triangle edges and two further lines that connect opposite triangle vertices but partly are not plane lines of curvature. The three ends coincide in their triangle vertices.

Both surface patches may be continued with the aid of the twofold axes forming the triangle pairs (*cf.* Fig. 6). The free boundaries must be chosen such that the spouts of neighbouring catenoids stick together and the free boundaries of the catenoids with three ends coincide.

The resulting minimal surfaces have the same inherent symmetry *I*4/*mcm*-*P*4/*mbm* as the *R*2 surfaces and, therefore, they are complementary to *R*2 surfaces and will be designated *C*(*R*2). As has been shown before they are complementary also to *MC*6 and *MC*7 surfaces (Koch & Fischer, 1989). Their genus is comparatively high, namely 25, whereas the genus of *R*2, *MC*6 and *MC*7 surfaces is only 9.

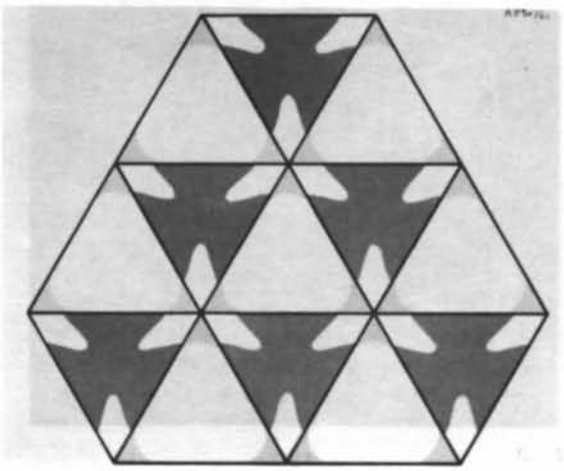


Fig. 5. Part of a *C*(*H*) surface spanned by two adjacent nets of twofold axes.

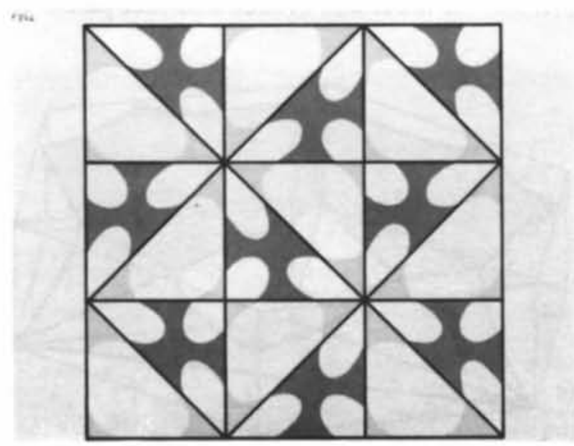


Fig. 6. Part of a *C*(*R*2) surface spanned by two adjacent nets of twofold axes.

### 3. Minimal balance surfaces *C*(*R*3)

*R*3 surfaces (Schoen, 1970) have inherent symmetry *P*6/*mcc*-*P*6/*m*. Their linear skeletal nets consist also of parallel plane triangular nets (angles: 30, 60, 90°) stacked directly upon each other. Again two kinds of triangle pairs exist within the linear skeletal net of an *R*3 surface giving rise to two kinds of surface patches with symmetry *m*.., namely catenoids and others consisting of three disc-like fragments which coincide in the vertices of the triangles. All three fragments have symmetry *m*.. but differ in their shape. As for *R*2 surfaces each fragment is bounded by two triangle edges and two additional free boundary lines, *e.g.* geodesics, connecting opposite triangle vertices.

In analogy to *C*(*H*) and *C*(*R*2) surfaces, more complicated surface patches with symmetry *m*.. may be formed which may be used to generate minimal balance surfaces of a second new family:

(1) Catenoids with three spout-like attachments are bounded by the triangles of a pair and by six additional free lines (*e.g.* geodesics). Three spouts form together a three-armed handle so that each catenoid is connected to five neighbouring ones. Catenoids which share the 90° vertices of their triangles are connected twice in analogy to *C*(*R*2) surfaces.

(2) Catenoids with three ends may be formed, too. Their three different boundaries correspond to those of the second kind of patches of *R*3 surfaces.

The resulting minimal balance surfaces have the same inherent symmetry *P*6/*mcc*-*P*6/*m* as *R*3 surfaces. They are complementary to *R*3 surfaces and will therefore be designated *C*(*R*3) (*cf.* Fig. 7). In addition, *C*(*R*3) surfaces are complementary to *MC*2, *MC*3 and *MC*4 surfaces (Koch & Fischer, 1989). Their genus is very high, namely 37, whereas the genus of the said complementary surfaces is only 13.

### 4. Minimal balance surfaces *tC*(*P*) and *oC*(*P*)

*tP* and *oP* surfaces may be regarded as tetragonally or orthorhombically distorted cubic *P* surfaces (Schoen, 1970). Their inherent symmetry is *I*4/*mmm*-*P*4/*mmm* and *Fmmm*-*Cmmm*, respectively. Infinite sets of parallel plane square (or rectangular) nets stacked directly upon each other form the respective linear skeletal nets. These nets contain two kinds of pairs of squares (or rectangles) with respect to a *tP* (*oP*) surface. Pairs of one kind correspond to catenoid-like surface patches, those of the other kind to surface patches consisting of four disc-like fragments each. A fragment is bounded by two quadrangle edges and by two further lines which are - in the case of tegragonal symmetry - plane lines of curvature. Adjacent fragments share two vertices of the quadrangles. The symmetry of the surface patches is 4/*mmm* for *tP* and *mmm* for *oP* surfaces.

The hexagonal prisms described above for *H* and *C*(*H*) surfaces correspond to tetragonal prisms that enclose *tP* surface patches. The rectangular prism faces are formed by mirror planes .*m*.;, the square faces contain the square nets of twofold axes. The vertices of the square nets coincide with the midpoints of the edges of the square prism faces. All boundaries of the catenoid-like surface patches refer to the square prism faces; the other surface patches show eight additional boundaries, two of them on each rectangular prism face. Adjacent prisms share entire rectangular faces, but only one quarter of their square faces.

In analogy to the derivation of *C*(*H*), *C*(*R*2) and *C*(*R*3) surfaces one may construct patches of surfaces that are complementary to *tP* or *oP* surfaces and show the same inherent symmetry:

(1) The catenoid-like surface patches give rise to more complicated ones that can be imagined as catenoids with four spouts attached. Their symmetry is 4/*mmm* and *mmm*, respectively, that of the spouts is *m*.*m*2 in the tetragonal case and 2*mm* or *m*2*m* in the orthorhombic case. For tetragonal surfaces each spout is bounded by two plane lines of curvature on two neighbouring prism faces. Four spouts belonging to four neighbouring catenoids are united to a four-armed handle with symmetry 4/*mmm* or *mmm*, respectively. As a consequence, each catenoid is connected to eight neighbouring ones *via* four four-armed handles. Four of these catenoids share vertices of the quadrangular nets with the original one and are connected twice. The other four have a larger distance and are connected only once.

(2) The surface patches of *tP* and *oP* surfaces made up from four fragments give rise to more complicated ones, the inner parts of which are similar to catenoids with four ends. The boundaries of these ends correspond to the boundaries of the fragments.

Both kinds of surface patches result in minimal balance surfaces which, on the one hand, are complementary to *tP* (or *oP*) surfaces and which, on the other hand, may be regarded as tetragonally (or

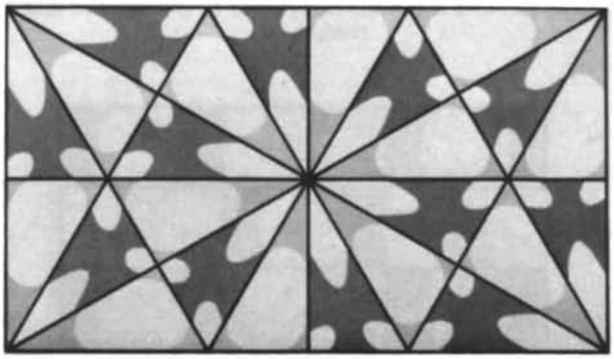


Fig. 7. Part of a *C*(*R*3) surface spanned by two adjacent nets of twofold axes.

orthorhombically) distorted $C(P)$ surfaces. They will therefore be designated $tC(P)$ (*cf.* Fig. 8) and $oC(P)$. These surfaces are, in addition, complementary to $MC5$ or $oMC5$ surfaces. The possibility of tetragonal or orthorhombic deformation of $C(P)$ surfaces has not been mentioned by Schoen (1970).

## 5. Minimal balance surfaces *PT*

The catenoid-like surface patches of *oP* surfaces allow a second possibility of constructing new surface patches. Instead of four spouts one may attach only two spouts to each catenoid. Thereby the symmetry *mmm* of the surface patch has to be preserved. Such a spout is bounded by one closed plane line of curvature referring to a mirror plane *m*.. or .*m*.. Two spouts are combined to a handle. Then each catenoid is connected by handles to two other catenoids which do not share vertices of the rectangular nets with the original one. The set of all catenoids connected by such handles is one-dimensionally infinite. It may be imagined as a perforated tube, the holes of which are formed by the ends of the original catenoids.

The catenoids with two spout-like attachments are the surface patches for a new family of minimal balance surfaces designated *PT* (*cf.* Fig. 9). As all

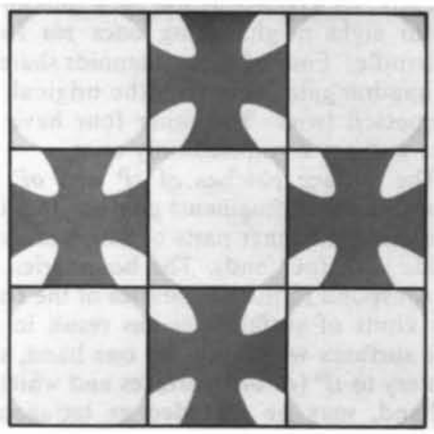


Fig. 8. Part of a $tC(P)$ surface spanned by two adjacent nets of twofold axes.

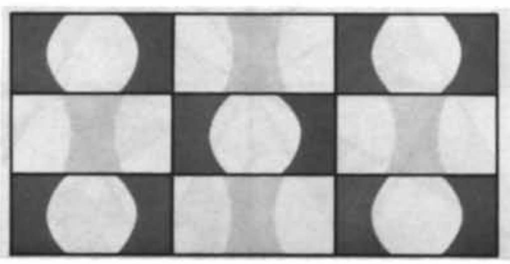


Fig. 9. Part of a *PT* surface spanned by two adjacent nets of twofold axes.

perforated tubes of a surface run parallel, the inherent symmetry of a *PT* surface is orthorhombic, namely *Fmmm-Cmmm*, regardless of whether its linear skeletal net consists of parallel square or rectangular nets. The genus of *PT* surfaces is 5. They are complementary to *oP*, $oMC5$ and $oC(P)$ surfaces.

## 6. Common properties

A survey of the minimal balance surfaces described in this paper is given in Table 1. The first column displays the symbol. In the second column the inherent symmetry of the surfaces is described by a group-subgroup pair of space groups with index 2. In all cases this inherent symmetry is the same as for the corresponding complementary surfaces built up from catenoid-like surface patches. As two surfaces with identical inherent symmetry also coincide in all other group-subgroup pairs compatible with these surfaces it is not necessary to repeat the information listed for surfaces with catenoid-like surface patches (Koch & Fischer, 1988). Column 3 gives the type of plane nets formed by the twofold axes of the generating linear net. The genus of the surfaces is listed in column 4.

Minimal surfaces with linear skeletal nets that disintegrate into parallel plane nets of twofold axes may be grouped into three classes depending on the surface patches that result from cutting the surfaces along all the twofold axes of their linear skeletal nets:

(1) The surface patches may be finite. Examples are catenoids, branched catenoids and multiple catenoids. The symmetry of such surface patches is a point group.

(2) The surface patches may be one-dimensionally infinite. Examples are strip-like surface patches (Fischer & Koch, 1989*b*) and surface patches that look like perforated tubes, as described above for *PT* surfaces. The symmetry of such a surface patch is a rod group in both cases.

(3) The surface patches may be two-dimensionally infinite. This is the case for all other families of minimal balance surfaces described within this paper. The symmetry of such a surface patch is a layer group.

Column 5 describes the symmetry of such infinite surface patches, all boundaries of which are twofold rotation axes. The layer- and rod-group symbols are chosen according to a proposition of Bohm & Dornberger-Schiff (1967).

The last column displays the point-group symmetry of the finite surface patches as described above. In addition to the twofold axes these surface patches are bounded by plane lines of curvature [$C(H)$, $tC(P)$, *PT*] or by more general lines, *e.g.* geodesics.

In analogy to *H*, *R*2, *R*3, *tP* and *oP* surfaces two minimal surfaces of the families listed in Table 1 are complementary to each other. They can be mapped onto one another by a reflection at a mirror plane through one of the nets of twofold axes.

Table 1. *Minimal balance surfaces, built up from catenoids with two, three or four spout-like attachments*

| Minimal balance surface | Group–subgroup pair | Nets of twofold axes | Genus | Symmetry of surface patches: Infinite | Symmetry of surface patches: Finite |
|---|---|---|---|---|---|
| $C(H)$ | $P6_3/mmc$-$P\bar{6}m2$ | $6^3$ | 7 | $P(\bar{6})m2$ | $\bar{6}m2$ |
| $C(R2)$ | $I4/mcm$-$P4/mbm$ | $48^2$ | 25 | $P(4/m)bm$ | $m.m2$ |
| $C(R3)$ | $P6/mcc$-$P6/m$ | 46.12 | 37 | $P(6/m)11$ | $m..$ |
| $tC(P)$ | $I4/mmm$-$P4/mmm$ | $4^4$ | 9 | $P(4/m)mm$ | $4/mmm$ |
| $oC(P)$ | $Fmmm$-$Cmmm$ | $4^4$ | 9 | $Cmm(m)$ | $mmm$ |
| $PT$ | $Fmmm$-$Cmmm$ | $4^4$ | 5 | $Cm(mm)$ | $mmm$ |

The existence of $C(H)$, $tC(P)$ and $PT$ surfaces can be proved by soap-film experiments. For $C(R2)$, $C(R3)$ and $oC(P)$ surfaces such experiments are impossible because of the absence of mirror planes that bound the finite surface patches. Probably $C(H)$, $C(R2)$, $C(R3)$ and $tC(P)$ surfaces exist only within a certain range of axial ratios $(c/a)_{\min} \leq c/a \leq (c/a)_{\max}$. The soap-film experiments suggest that $(c/a)_{\max}$ is larger for $C(H)$ and $tC(P)$ surfaces than for $H$ and $tP$ surfaces, *i.e.* the handles connecting the catenoids stabilize the minimal surfaces for large $c/a$ values. For orthorhombic surfaces the ratios $b/a$ and $c/a$ must be examined. $b/a$ describes the shape of the rectangles and $c/a$ the distance between the nets. In the case of the $PT$ surfaces the soap-film experiment shows that handles in the $a$ direction are stable only for $b/a \geq (b/a)_{\min} > 1$. $PT$ surfaces, therefore, are incompatible with square nets.

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# A Full-Symmetry Translation Function Based on Electron Density*

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## Abstract

A method for positioning an oriented fragment within the unit cell is presented. It is based on a correlation between a model and observed data which is performed in Fourier rather than Patterson space. Symmetry-related molecules are located in the electron density map calculated in space group $P1$, with the phases derived from a model that is correctly oriented but arbitrarily positioned in the unit cell. It is shown that considering all symmetry elements simultaneously substantially increases the sensitivity of the method and makes it less susceptible to the errors in the model. The procedure also automatically incorporates a penalty for the overlap of symmetry-related molecules, and the stringency of this requirement is easily modified. The method has been tested on two different proteins and the results compare favorably with other translation functions.

## Introduction

Analysis of the architecture of proteins with known 3D structures (*e.g.* Rossmann & Argos, 1976; Richardson, 1977, 1981; Chotia, 1984; Janin & Chotia, 1980; Chotia, Levitt & Richardson, 1981) indicates that their folding pattern is conserved to a much higher degree than their amino-acid sequence, and suggests that the number of different structural motifs (patterns of folding units of a polypeptide chain) in globular proteins is relatively limited. Knowing the amino-acid sequence of a particular protein, one can obtain some information about its structure from a possible sequence homology to other proteins with known structures. This knowledge can be utilized either for building a model of the protein (*e.g.* Blundell,

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