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Notes of a protein crystallographer: the beauty of rose windows and the different meanings of symmetry

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To the architects, draughtsmen, stonemasons and stained-glass workers of the Middle Ages who gave us an enduring and incomparable legacy of their view of the cosmos.

The brief book *Symmetry* written by Professor Hermann Weyl (1885–1955) in 1952 is an unsurpassed gem of scope and conciseness, describing the concept of symmetry and its presence in various forms of art, and the abstract concept of symmetry and conservation in the physical world. Beginning with the presence of bilateral symmetry in the early manifestations of Sumerian art (2700 BC), he guides the reader through the intricacies of different kinds of symmetry, culminating in crystallographic symmetry (Weyl, 1952).

I have read many sections of the book several times, and even now I still find insightful and thought-provoking observations. Among the brief detours found on the pages of this unique book, there is one that I would like to highlight here: the connection between cyclic symmetry and the magnificent 'rose windows' present in the Gothic cathedrals of Europe. I quote (p. 58):

> Magnificent examples of such central plane symmetry are provided by the rose windows of Gothic cathedrals with their brilliant-colored glasswork.

Unaware of this brief reference, this connection struck me about two years ago while again visiting the Cathedral of Burgos, Spain, displaying in one of its façades a unique 20-fold pattern (Fig. 1). Like many people, I have been fascinated by the beauty of the rose windows for many years, but as a trained crystallographer I could not avoid counting the number of 'rays' or 'spokes' radiating from the center, seeking to characterize their symmetry, and recently I have begun to look at the various windows systematically. Soon thereafter, I found the superb compendium of images available in the book *The Rose Window: Splendor and Symbol* by Painton Cowen (Cowen, 2005), as well as the accompanying website http://www.therosewindow.com. The combination of the book and the electronic resource provides an amazing collection of images merged with a historical overview, successive evolution, construction details and iconographic meaning present in the stained glass of several hundreds of windows. The magnificent images are inspiring and can be used to introduce examples and the notions of cyclic planar symmetry to students and to the public at large.

Painton Cowen's work also presents among the notes an interesting table (Cowen, 2005, p. 273) with a survey of the basic geometry of the 524 windows that he has studied. I have taken the liberty of plotting these data in a histogram fashion to present the frequency of the different basic geometrical patterns present (Fig. 2). The results clearly document that the most common arrangements are based on four, six, eight, 12 or 16 repetitions around the central point. Those based on five-, ten- or 20-fold patterns are rather uncommon. A possible reason for this is the inherent difficulty of inscribing a regular pentagon (and related even multiples) in the circumference using the tools available to the artisans of the time, namely a compass and the straight edge. Incidentally, Euclid had shown in his *Elements* (third century BC) that it was possible to divide the circle into two, three, four, five, six, eight and 12 parts using only those tools; importantly, not seven, nine, 11 or 13 or more parts. A complete discussion of this subtle difference is related to studies by the great mathematician C. F. Gauss (1777–1855) and his discovery that it was also possible to divide the circle into 17 parts when he was only a young lad of 19. This intriguing result deserves an extensive discussion that we can revisit some other time.

I wish to use a few examples of rose windows from Cowen's images and my own personal collection to illustrate several types of cyclic symmetry and how the different types of symmetry can convey a different message to the viewer. This might have been the intent of the artists who designed them, but I challenge the readers to judge for themselves the reaction that these images provoke in them.

As indicated, the pattern based on 12 rays (cyclic 12-fold repeat) is one of the most common patterns. The number 12 has many resonances in human culture such as months of the year, zodiac symbols and, in the Christian context, the number of apostles; thus, it is easy to understand the frequent presence of this pattern. However, a 12-fold repeated pattern can be presented in two radically different ways that can be related to two distinct types of symmetry. These are illustrated in Fig. 3. The first presents the most common division of the circle into 12 parts, with the left half balanced by the corresponding right part related by bilateral (or mirror) symmetry (D_{12}). A technical issue should also be discussed here. In the plane, the bilateral symmetry is also accomplished by the presence of twofold axes (180° rotations) perpendicular to and intersecting the main axis at regular intervals ($360/n$), described by the 'dihedral' planar symmetry groups D_n, with n being the high symmetry axis (n = 2, 3, 4, 5, 6, ...). The presence of these axes is important if a 'balanced' composition is to be achieved with an asymmetrical object or by the interlacing of the main motif.

The second (Fig. 3*b*) is certainly a rare pattern that cannot be discerned by the classification in Cowen's catalog. It presents a wheel (or spiral, as it is described) of 12 curved leaves or 'mouchettes' packed around the central point. Neither the reflection (mirror symmetry) nor the twofold repeat are present in the plane. Thus, the resulting image is strikingly different: only cyclic C_{12} symmetry. The immediate image that comes to mind is that of a rotating windmill or vortex, spinning unrelentingly as in the flow of time or life or even a wheel of fortune. Possibly the 12 petals might symbolize the months of the year or the flow of time, but without further investigation it is difficult to come to a definite conclusion.

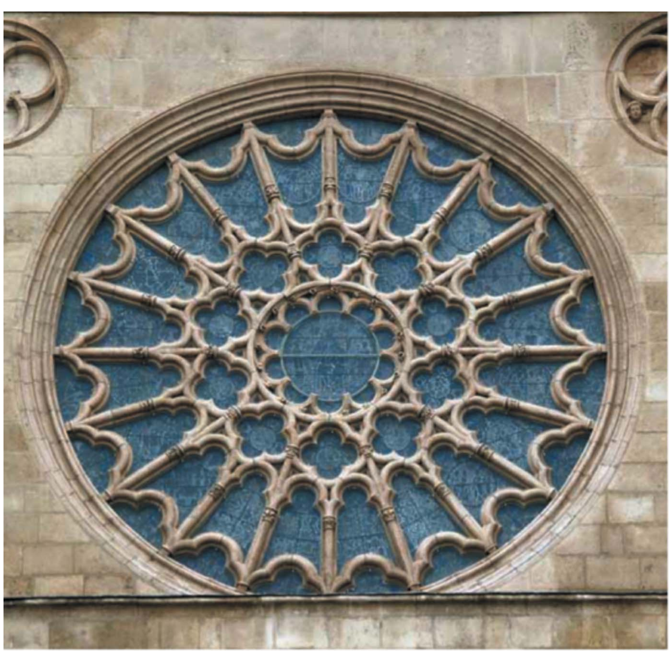


Figure 1
Rose window on the south entrance (Puerta del Sarmental) of the Burgos cathedral in Northern Spain. The 20-fold pattern is rather rare. The symmetry of this rose window is C_{10v} (or 10*mm*), consisting of a tenfold central symmetry (inner circle) and mirror planes of symmetry duplicating each 'leaf' on the other side of each of the ten radial lines. Overall, the left side is balanced by a symmetrical equivalent on the right side. Image from the personal collection of the author.

It is important to emphasize now that the stone tracery of the 'rose window' provides *only* the geometrical (symmetrical) framework; the content is provided by the stained-glass windows, which are another marvel on their own (see also the discussion by Painton Cowen in the resources mentioned above; Cowen, 2005). Indeed, two windows with the same overall symmetrical pattern can be decorated with a different stained-glass content, providing a different meaning. The stained-glass material is provided by the amorphous structure of quartz plus heavy metals and ions.

In this context, it is significant to highlight the inimitable window of the Cathedral in Lausanne, Switzerland. This masterpiece was designed and built in 1220–1235 by Pierre d'Arrass, although it was probably planned as early as 1205. It is over 8 m in diameter and is based on a fourfold repeated pattern around a central circle (Fig. 4*a*) with a bilateral symmetry balance (C_{4v} or 4*mm*). As remarkable as the stone tracery is, I would like to discuss the content included in the stained-glass work briefly. Further details can be found within the rose-window website (http://www.therosewindow.com/pilot/Others/Lausanne-Frame.htm), and I encourage the reader to explore the individual symmetrical groupings around the central square (Fig. 4*b*) to visualize the meaning of each individual stained glass panel and the different clusters.

This window represents an *Imago Mundi* of the medieval world, a graphical summary of all knowledge of the universe. Possibly, the layout was inspired by diagrams showing the cycle of the year from a 12th century manuscript from Kloster Zwielfalten, Swabia, as suggested by Cowen (2005). Rotating about the central circle showing 'God the Father' (A) there

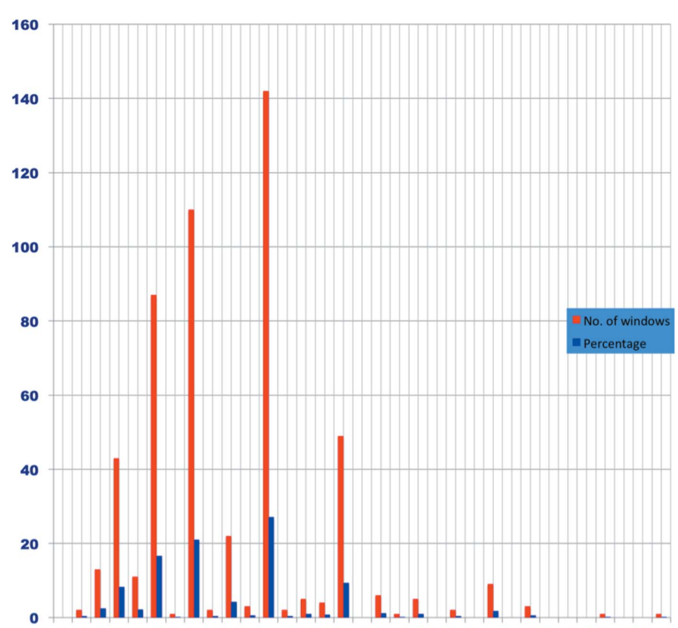


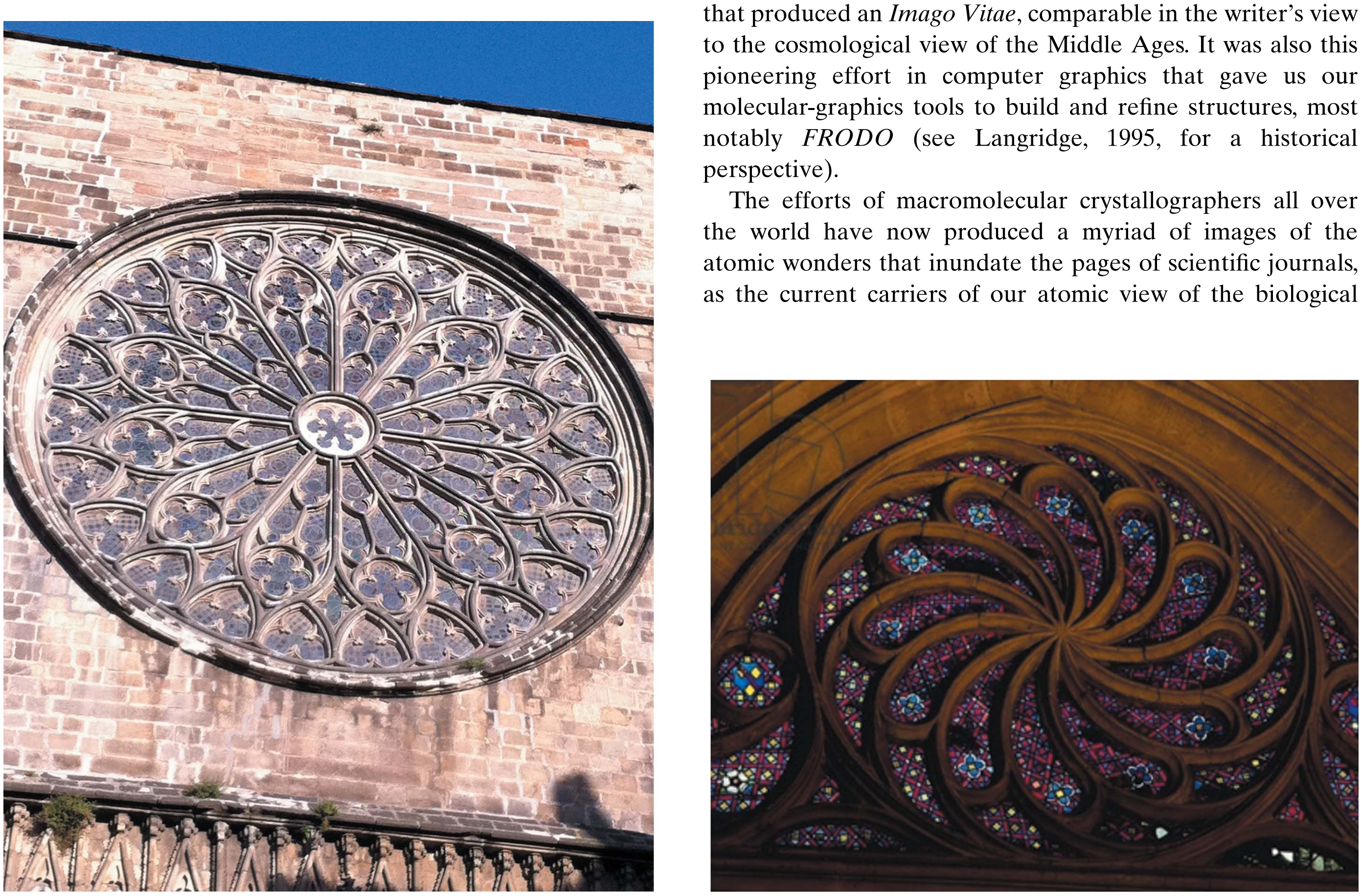
Figure 2
Summary histogram of the data presented in Cowen's survey of 524 rose windows. The plot represents the number of windows in red (ordinate) *versus* the number of 'rays' or 'spokes' (abscissa). The data were extracted from *The Rose Window: Splendor and Symbol* by Cowen (2005). Blue is the histogram of percentages (Cowen, 2005, p. 273). Note: the original table cites a total of 522 windows, but the total is actually 524.

are four circles in the central square representing the Creation (Figs. 4*a* and 4*b*). Clockwise around this central square there are four semicircles (B–E) representing the seasons and the corresponding months around them. The alternating circles encircling these (F–I) contain the four elements of antiquity (earth, water, air and fire) and the zodiac signs. Illustrating also the geography of the biblical world, the four square corners (J–M) include the four rivers of Paradise and mythical worlds with imaginary creatures (*e.g.* Acephali: creatures with no head and eyes in their chest; left of J). Finally, the outermost eight trefoils (N–U) represent the eights winds of the cosmos (Figs. 4*a* and 4*b*; Cowen, 2005).

What can we offer now to counterbalance this masterpiece of the Middle Ages? What can we present as iconic images of our scientific view of the cosmos nowadays? We do not currently build many cathedrals, with an exception made for the Sagrada Familia in Barcelona, Spain, which was originally designed by the Catalan architect Antonio Gaudí at the beginning of the 20th century and the construction of which is still continuing. Our design tools are no longer the compass and straight edge but computers and electronic images. Readers can select their own iconic representations of the world that we inhabit in our time, but in this context and as a macromolecular crystallographer and structural biologist, my choice is the 'atomic rose window' that appeared on the cover of *Science* on 13 February 1981 (Fig. 5*a*). An important clarification is due here. The image of the atomic structure presented in this issue of *Science* was of a three-dimensional object (a helix), not a planar object like the 'rose windows'; however, the orientation chosen and the tenfold symmetry of the object itself make the analogy very appealing.

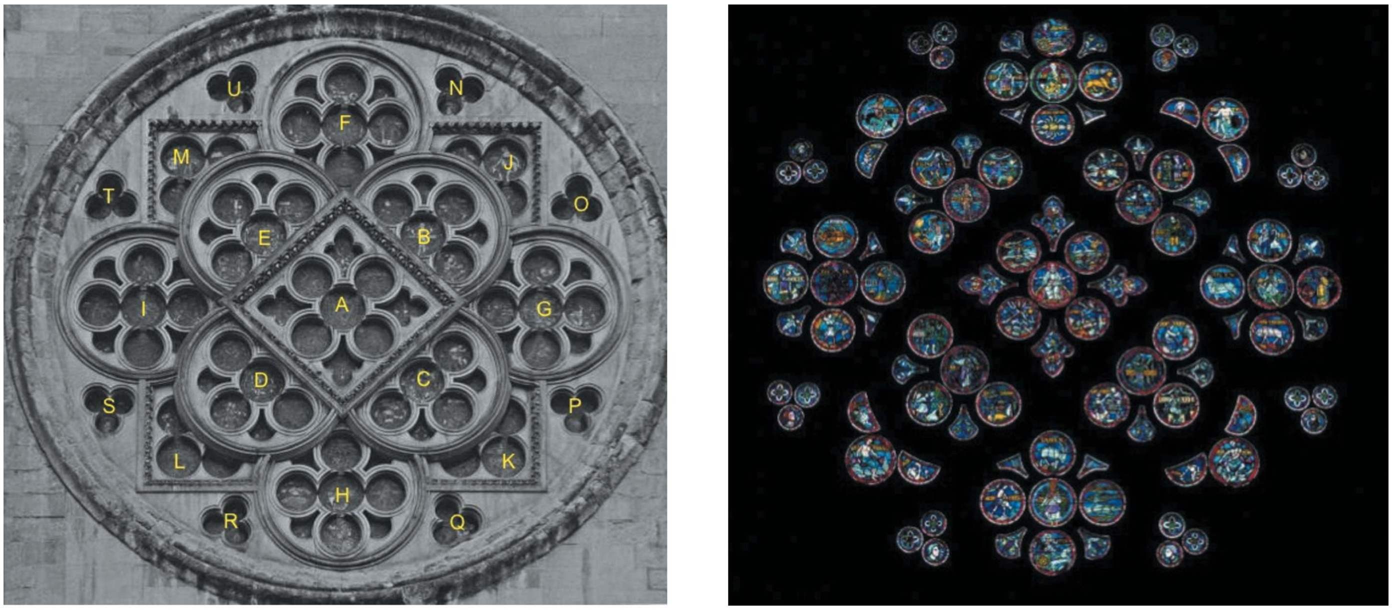
Those were times when the computer and computer graphics were beginning to have an impact on analysis of the structure and function of biological macromolecules at the atomic level, pioneering work that has been recognized recently by the Nobel committee with the award of the Nobel prize in Chemistry to Karplus, Levitt and Warshel in 2013. At the time, the ground-breaking work of Langridge, Ferrin, Kuntz, Connolly and others in molecular graphics succeeded in integrating the structural knowledge, beauty and mystique of the structure of B-DNA into an 'electronic rose window' that produced an *Imago Vitae*, comparable in the writer's view to the cosmological view of the Middle Ages. It was also this pioneering effort in computer graphics that gave us our molecular-graphics tools to build and refine structures, most notably *FRODO* (see Langridge, 1995, for a historical perspective).

The efforts of macromolecular crystallographers all over the world have now produced a myriad of images of the atomic wonders that inundate the pages of scientific journals, as the current carriers of our atomic view of the biological



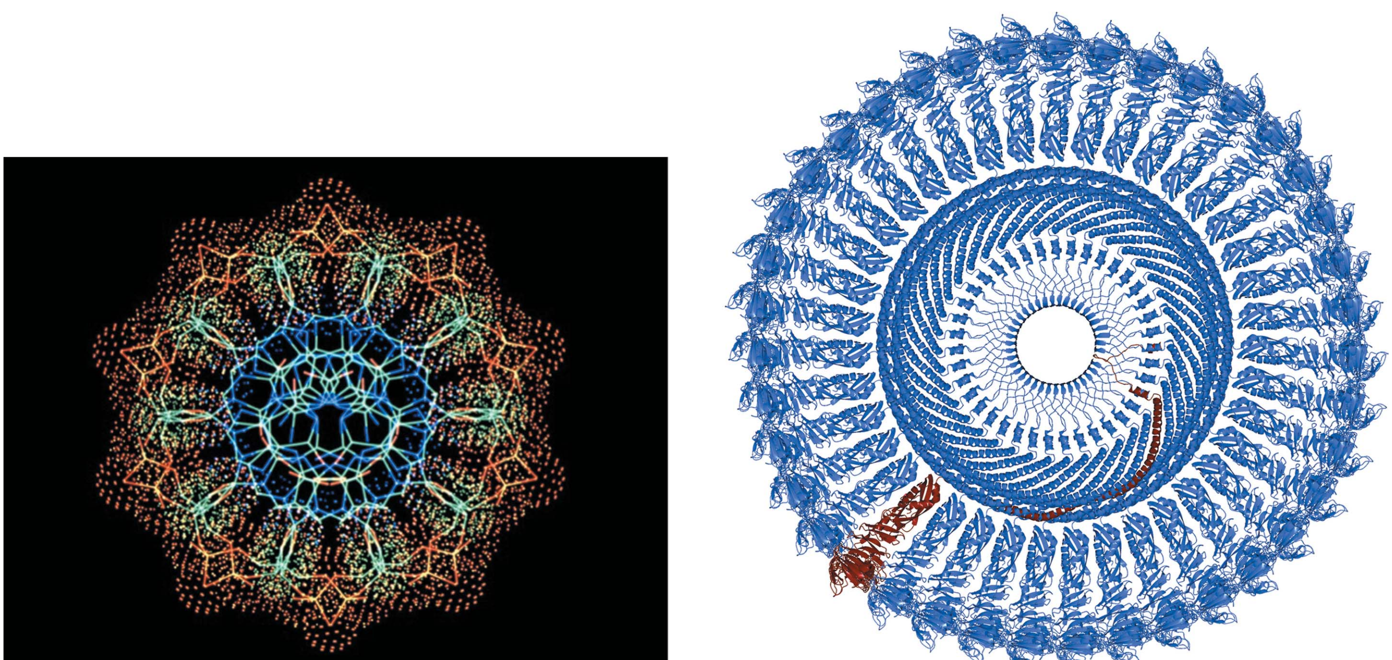
(*a*) (*b*)

Figure 3
Two examples of cyclic 12-fold symmetry in rose windows with two radically different arrangements. (*a*) View of the rose window in the main façade of the church of Santa María del Pi in the Cita Vella of Barcelona. The construction and symmetry is very similar to that found in the upper rose window at the main entrance to Reims Cathedral in France. From the central sixfold repeat the number of 'rays' doubles (left to right) as it expands out to 12 'petals' and contains 24 curved triangles on the outmost edge. Ignoring the innermost hexagon, the rose has symmetry C_{12v} (12*mm*). Image from the author's personal collection. (*b*) View of the rose window inside the chapel of the Bourbon in the cathedral of Lyon, France. Image obtained from the website http://www.therosewindow.com. The pattern exhibits only cyclic 12-fold symmetry (C_{12}). Further details can be found on the website and also in the book by Cowen (2005). Reproduced from the website with permission. Courtesy of P. Cowen.



(*a*) (*b*)

Figure 4
Views of the rose window of Lausanne cathedral in Switzerland: *Imago Mundi.* (*a*) External view of the stone tracery (c.1205). The design is essentially tetragonal, but the alternating elements of circles and squares add variety within a perfectly balanced composition (C_{4v}, or 4*mm*). The various fourfold encircling motifs are labeled clockwise as discussed in the text, A, B–E, F–I, J–M and N–U, and refer to the stained-glass content explained in (*b*). (*b*) Internal view with the images of the stained glass (c.1230). The central square (A) representing the Creation is surrounded by four semicircles (B–E) representing the seasons and months of the year. Alternating, there are full circles (F–I) with images relating to the four elements of antiquity (earth, water, air and fire) and zodiac signs. J–M are used to depict the rivers of Paradise and the mythic lands beyond the confines of the known world. Surrounding the world are the eight winds of the cosmos (N–U). Reproduced with permission from the website http://www.therosewindow.com and adapted for description. Courtesy of P. Cowen. See the website for details.



(*a*) (*b*)

Figure 5
Iconic images of the biological atomic world: *Image Vitae*. (*a*) The B-DNA 'atomic rose window'. The structure of DNA is undoubtedly one of the icons of the atomic description of the biological world in the 20th century. It has been presented and illustrated in multiple images and contexts. The suggestive 'atomic rose window' or 'electronic rose window' presented by Langridge and coworkers using early computer graphics (Langridge *et al.* 1981) is particularly relevant. From Langridge *et al.* (1981). Reprinted with permission from AAAS. (*b*) The 39-fold view of the vault structure. Going beyond what Gauss demonstrated to be possible geometrically, vaults present a cylindrical enclosure with 39 2 (D_{39}) symmetry (Tanaka *et al.*, 2009). The red tracings indicate one polypeptide chain that generates the enclosure by the close point-group symmetry; the perpendicular twofold repeats generate the top and bottom of the cylindrical enclosure. View along the higher symmetry axis. High-resolution image courtesy of Professor T. Tsukihara, H. Tanaka and colleagues.

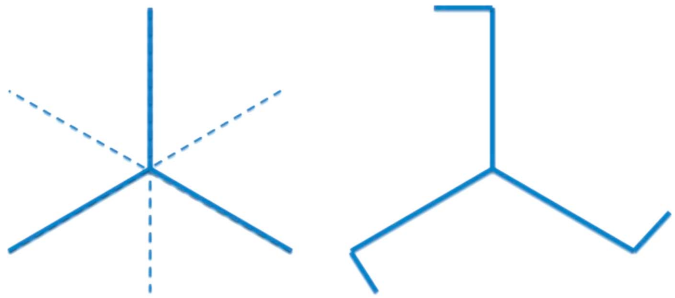


Figure 6
Rotational *versus* dihedral symmetry. The critical difference is shown between cyclic patterns containing rotational combined with dihedral symmetry (left) and the same order of cyclic symmetry only (right), making the latter figure unbalanced and suggesting motion/rotation. This is illustrated for the simplest cyclic symmetry, order equal to 3. The correct symmetry-group symbols are D_3 (or 32) and C_3 (or 3), respectively. Tripod (left) *versus* triquetrum (right). Dashed lines indicate the positions and directions of the additional twofolds perpendicular to the main symmetry axis of order 3. The additional symmetry produces a 'balanced' figure that will repeat any motif 'left and right'.

world. I would like to add one more to demonstrate that the atomic ingenuity of nature has surpassed even the mathematical logic of Gauss by inventing a cylindrical enclosure (vault) with 39 protein units in a close circular arrangement with a 'top' and 'bottom' (D_{39} or 39 2 symmetry), the name of which also refers to one of the architectural elements of cathedrals (Fig. 5*b*). The structure and some of the details of the function of these fascinating vault-like particles have been revealed by the groups of Tsukihara and coworkers in Japan (Tanaka *et al.*, 2009) and Fita, Verdaguer and coworkers in Barcelona, Spain (Querol-Audí *et al.*, 2009; Casañas *et al.*, 2013).

After these brief examples, we can go back to the inimitable book by Professor Weyl, in which he discusses the meaning of symmetry and alludes to the difference in content of cyclic patterns containing bilateral symmetry *versus* those containing only rotational arrangements. He quotes Dagobert Frey in an article entitled *On the Problem of Symmetry in Art* (Weyl, 1952),

> Symmetry signifies rest and binding, asymmetry motion and loosening, the one order and law, the other arbitrariness and accident, the one formal rigidity and constraint, the other life, play and freedom

(included in the book *Studium Generale*).

To illustrate this point later in the book, he compares the image of the tripod (the simplest figure with rotational symmetry, $n = 3$; Fig. 6, left) with the corresponding image resulting when one adds little flags onto the arms to obtain the triquetum (Fig. 6, right), thus breaking the bilateral symmetry. This resulting figure is an old magic symbol that was used by the Greeks with Medusa's head in the center to represent the three-cornered Sicily. This symbol has now been revived and is included in the flag of Sicily (http://en.wikipedia.org/wiki/File:Flag_of_Sicily.svg). The exact word used by Weyl is not found in most dictionaries, but related words such as 'triskelion' and 'triskele' are rather common, all characterized by a threefold pattern without the balancing bilateral symmetry (C_3). This type of basic three-lobed symbol is common in Celtic culture as a 'triple spiral' and represents primordial motion and change, although it was later used to represent the 'Trinity' and other religious concepts. I should add that in flowers both approximately cyclic (*Vinca herbacea*) and closely dihedral (genus *Geranium*) pentagonal forms exist, as documented by Weyl (Weyl, 1952; p. 66). At the atomic level, point-group symmetry containing mirror symmetries is not possible in biological molecules.

These reflections illustrate how various symmetrical figures and entities that are part of our world, and which can be described by the rigorous framework of group theory in mathematics, have been used throughout history to convey different thoughts, insights and perceptions of the artist (or the scientist) as a draughtsman and executor of the cosmological view of the times. Both artists and scientists will continue to create and unveil novel symbols of their times to illuminate and enrich the world in which we all live. Further research efforts and artistic ingenuity will carry the torch of our predecessors.

The comments and insights on earlier versions of the manuscript by Dr Ignacio Fita are greatly appreciated. The original image at high resolution of the structure of the rat liver vault MVP from Professor Tsukihara and coworkers is greatly appreciated. This essay is written by the author on behalf of the CrysAC of which he is a member but the opinions expressed are his own.

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