

SYMMETRY: CULTURE & SCIENCE

REFLECTIONS ON ROTATIONS: CONNECTIONS AND NOTATIONS

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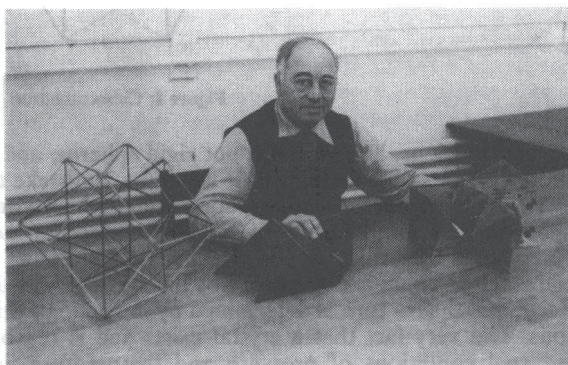
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QUESTION 1

what is
symmetry?

Crystals are symmetrical because they are made up out of identical building blocks (atoms or ions), which tend to surround themselves with identical environments. If we call the distance between a_i an ion or atom of type a and b_j , an ion or atom of type b , $r_{ij}(a,b)$, and the crystal constitutes atoms or ions of types a , b , c , d ... etc., then for any pair (a,b) as many as possible of the distances $r_{ij}(a,b)$ will be identical.

This principle, the *Vector Equilibrium Principle*, accounts for a large number of inorganic crystalline configurations (Loeb 1970). As a special case, when there is but a single constituent, a , for instance copper atoms, then any atom a_i may be surrounded by at most twelve other atoms a_j , located at three vertices of a cuboctahedron (Figure 1), whose center is at the location of atom a_i . (We shall call these twelve the *vertical* atoms.) Each of the vertical atoms is equidistant from

four other verticial atoms a_j as well as from the central atom a_i . When each of the vertical ions or atoms is in turn surrounded identically by twelve neighbors, and this process is continued indefinitely, a configuration is generated which has become known as the (cubically) close-packed lattice. R. Buckminster Fuller has called the cuboctahedron *Vector Equilibrium* because of the equality of all the distances from the vertices to the center and to four other vertices.

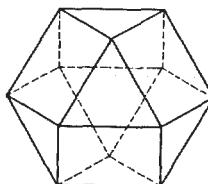


Figure 1: Cuboctahedron

Atoms and ions, however, are not rigid spheres, and the success of the rigid sphere model is somewhat fortuitous. It would be a mistake to deduce from the fact that the cubically close-packed configuration is quite common, that atoms and ions are rigid spheres: they are, in point of fact highly concentrated positive charges, the nuclei, surrounded by diffuse clouds of negative charge, the electrons. The configuration of the electron cloud is determined by the symmetry of the electric field in which it finds itself, and that in turn is determined by the configuration of the surrounding atoms or ions. The very fact that a crystal exists and is reasonably stable under the existing external conditions of pressure and temperature, indicates that the Energy $\sum_{ij} V\{r_{ij}(a,b)\}$, is minimized. [We here assume that the total energy may be expressed as the sum of the separate pairwise interactive energies $V\{r_{ij}(a,b)\}$.

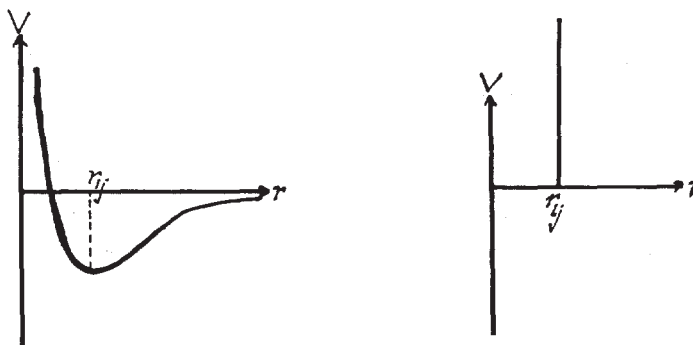


Figure 2a: Interaction potential for a stable pair of atoms or ions
Figure 2b: The same for two tangent rigid spheres

The potential energy of a pair of atoms or ions (a_i, b_j) is plotted in Figure 2a as a function of the distance between them, r . The equilibrium distance r_{ij} corresponds to the minimum value of V . For contrast, V is plotted as a function of r for two rigid spheres in Figure 2b. In the latter case a minimum-energy configuration is achieved when each sphere center is at distance r_{ij} from its twelve nearest neighbors. In the former case, as long as we ignore interactions between all but twelve nearest

neighbors, equilibrium would also occur when *each* atom or ion is at distance r_{ij} from twelve nearest neighbors, for we know that our three-dimensional space cannot accommodate more than twelve nearest neighbors in such an array.

Now suppose, however, that interactions between more distant atoms or ions would play a significant role. The interaction-energy between atoms or ions at larger distances than the equilibrium distance from each other would tend to destabilize the cuboctahedral configuration, because the more distant atoms or ions would attract each other (cf. Figure 2a). Thus it might be energetically more economical to bring more atoms into a configuration in which there are more than twelve *near*, although not *nearest* neighbors. Such a configuration is shown in Figure 3, a rhombic dodecahedron. If one ion or atom is at the center of this dodecahedron, then fourteen others will occupy its vertices; in turn, each of these vertexial ions or atoms may be at the center of an identical dodecahedron. When this algorithm is applied again, the so-called body-centered cubic lattice is generated, a configuration almost as common as the cubically close-packed one. Of the fourteen near neighbors, the eight nearest ones are at the vertices of a *cube* (hence the name of the lattice), whereas the six next-nearest ones are at the vertices of an octahedron: together these fourteen constitute the eight obtuse and six acute vertices of the rhombic dodecahedron. The six nearest neighbors are only 15% closer than the eight next-nearest neighbors in this configuration.

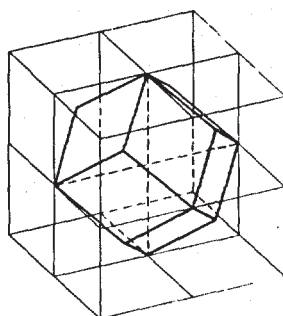


Figure 3: Rhombic Dodecahedron

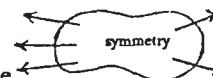
When we examine Figure 2a in the light of the body-centered configuration, we have to accept the fact that not all nearest and next-nearest neighbors may be at equilibrium distance. Thus we lose some energy, but this loss is offset to some extent by the greater number of neighbors to be accommodated in this configuration. The cost of placing neighbors at a less-than-optimal distance depends on how steeply the potential-energy curve in Figure 2a rises from its minimum. The steeper this rise is, the less economical this configuration will be in competition with the close-packed one.

We conclude that crystalline configurations result from a balance of counteracting forces. In our examples, the dependence of potential energy of interaction on separation distance had to be balanced against the properties of three-dimensional space which limit the numbers of nearest and next-nearest neighbors. Changes in such external conditions as pressure and temperature may shift this balance in one direction or the other, and cause changes in configuration known as *phase-shifts*. Many elements and compounds form simple crystals in the configurations related to cubically close-packed and body-centered lattices (cf. Loeb, op.cit.), but other metals and their alloys, for instance those containing manganese, have very complex

configurations, probably as a result of very delicate balances. Notably, the latter, complex crystals will also experience many phase shifts when external conditions are varied, with resulting shifts in the delicate balances, whereas the simpler configurations tend to be stable in the face of changes in external conditions.

Accordingly, symmetry in crystals is the result of the trend for as many identical building modules as possible to be identically surrounded, but their configuration is the result of a balance between forces which cannot all be simultaneously optimized. In particular, increase in temperature will also increase entropic randomization, with resulting crystalline imperfections. These imperfections are in some instances responsible for desirable characteristics such as malleability and semi-conductivity.

QUESTION 2



Above, reference was made to R. Buckminster Fuller's naming the cuboctahedron the *Vector Equilibrium*. Although Fuller is particularly known for his dome structures, *minimal* structures in the sense that they cover a maximum volume with a minimal area, it is remarkable that he should have been so interested in packing with *maximal* density.

Is the similarity between architectural structures designed by Fuller and the microstructures of viruses and inorganic crystal structures fundamental or coincidental? Although the forces may be of quite different natures, the space in which they act is the same, and the same constraints apply. At equilibrium, the potential energy will necessarily increase quadratically with displacement from equilibrium as long as that displacement is relatively small, regardless of the scale at which these forces act. And the constraints due to the properties of three-dimensional space will prevail, and favor the cuboctahedron and the rhombic dodecahedron, at either architectural or microscopic level. The repertoire of permitted configurations, though varied, is finite and limited.

A pattern is an ordered array, and structure is the expression of the interrelations between the members constituting an ordered array. Pattern recognition is the recognition of these underlying relationships; such recognition may be quite subjective. For example X-ray crystallographers are conditioned to relate their experimental results to a cubic framework whereas solid-state chemists will look for other polyhedra such as the cuboctahedron and the rhombic dodecahedron to understand why the atoms and ions form the patterns which they do. (Cf. Loeb, op.cit.)

The New England Transcendentalists of the nineteenth century believed strongly in underlying significant patterns in nature. The ability of a scientist to discriminate between significant and trivial patterns is a characteristic of genius. A grandnephew of transcendentalist Margaret Fuller, Buckminster Fuller attributed his own ability to discern the significant pattern to intuition. We have reason to believe that intuition may be non-verbalized knowledge. (Haughton & Loeb, 1964; Loeb & Haughton, 1965) In any case, one is not apt to discern a pattern unless one is thoroughly familiar with it. An illustration is the recent discovery of the molecule which was named *buckminsterfullerene*: the choice of this name is testimony to the familiarity with Fuller's dome structures which the discoverers enjoyed.

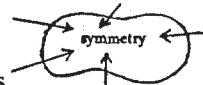
Mass production has been blamed for the creation of boring repetitions of identical structures in our environment. There is no need for such tedium. Nature has had

fewer than one hundred elements, and, using just carbon, oxygen, hydrogen and nitrogen has produced endless varieties of life. Gemstones of brilliant variety are constituted of relatively few different elements and frequently owe their distinctive color to small impurities or imperfections. It is not the modules but the way in which they are interconnected that gives us variety. Accordingly, designers and architects need to understand the way in which modules can or cannot be interconnected in order to create a maximum variety out of a minimum of different modules.

Yona Friedman has pointed out the substantial difference in the way we dress as a result of confection, the mass production of clothing. Whereas the well-dressed and well-heeled citizen used to have her or his attire tailor-made, confection has made clothing available in such variety of sizes and shapes, that we are now able to mix and match in a multiplicity of combinations, and with a moderate wardrobe are able to appear dressed differently at a large number of different events.

Intuition alone does not suffice to understand and exhaustively explore the way in which things interconnect. Abstract analysis and synthesis will extend one's spatial repertoire through the use of such parameters of spatial order as symmetry, connectivity and stability, which constitute the grammar of spatial structure much as harmony and counterpoint are part of musical grammar.

QUESTION 3



Hans Jaffé has observed that the environment in the Netherlands is entirely man-made: there are few if any remnants of wilderness. Jaffé feels that Mondriaan's abstract works reflect this Dutch landscape. Indeed, just as Mondriaan's *Broadway Boogie-woogie* with its prominent diagonal element refers to an aerial view of Manhattan, so his right-angled designs reflect the orthogonal features of the Dutch man-made landscape.

I am told by Art Historians that Mondriaan was a fine dancer. I already knew that, as my mother frequently danced with Mondriaan, but since some Art Historians tend to discredit so-called anecdotal evidence, one must be grateful for their authoritative confirmation. My grandfather was friendly with and had business dealings with Sal Slijper, Mondriaan's friend and collector of his work, and so it was that my mother as a teenager got to know the artist at the time of his first experiments with abstraction. Those were the heady times of the periodical *De Stijl*, and the first designs by the architect Rietveld. (Loeb & Loeb, 1986)

Recently some very trendy stores in the Netherlands have marketed copies of Rietveld's early chairs, but I have sat in an original one, in the kitchen of Rietveld's daughter. As a matter of fact, when I turned thirteen, and was given my own room, its furnishings included one of the first Breuer chairs and a set of Aalto chairs and a table. As I presently sit behind my computer in my Cambridge study, could I claim that those objects in far-away Amsterdam in a too distant past would still influence my present visual environment? Most assuredly I do, for I am looking at, and just sat in my Breuer chair: it endured war and transplantation, and its design is still valid and trendy.

When I turn to my right, I see on the wall two four-by-four tableaux of Delft tiles. I remember my grandfather in his garage (the car was parked somewhere else, about a twenty minutes' walk away), carefully matching corners and edges, attempting to recreate assemblies of tiles which centuries ago graced kitchens and dining rooms,

but since then were scattered, and in part destroyed. As grandfather was experimenting (I was about three years old), I was initially intrigued by the flowers, animals and persons portrayed on the tiles, but shortly I discovered something quite fascinating: each tile would have a little motif in each corner. An lo! when a correct match was achieved, four tiles would neatly fit together about a common corner, and that corner would be surrounded by a pretty, symmetrical rosette, made up of the corner motifs of the surrounding tiles.

It would be a good many years before I articulated this discovery into the implication of symmetry generated by an algorithm for putting multiples together (Loeb, 1971). But the very fact that I so clearly recall this experience from my fourth year indicates that this was a formative experience. My grandfather died when I was not quite nine years old, but I recall him always asking my arithmetic teacher how I was doing.

A biographical sketch of the Amsterdam architect Piet L. Kramer (Ed. Wim de Wit, 1983) states: "In 1923, he participated in the competition for the Bijenkorf department store in The Hague. Although not the winner, he was nevertheless given the commission; ...[the] design which was actually chosen by the jury, was considered too advanced by the patron. Kramer's Bijenkorf can be regarded as the last original Amsterdam School creation..." The patron was my grandfather and Piet Kramer became a friend of the family, and redesigned the bottom two floors of our own house. When, years later, I studied at the Amsterdam Muzieklyceum, Kramer's wife Bodi Rapp was one of my teachers. Patterns and mathematics were indeed part of my upbringing, and De Stijl, the Bauhaus and the Amsterdam School, characterized by geometric patterns, were always visible in my living environment.

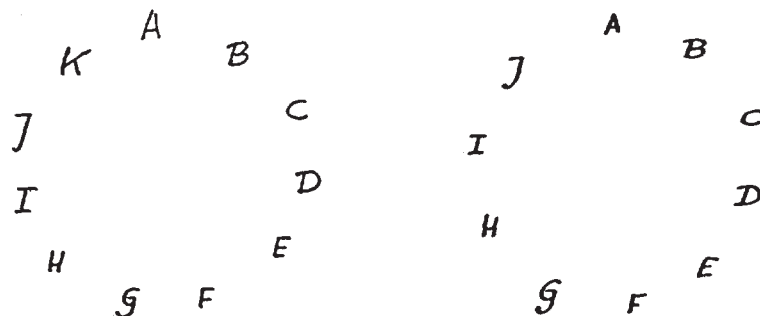


Figure 4: Polygonal representation of the teams in a soccer competition: a) The Division comprises an odd number of teams; b) The Division comprises an even number of teams.

In my 'teens I enthusiastically followed the soccer competitions, and before long became intrigued with the question how to schedule games between all teams during the limited number of Sundays available in the soccer season. Some of the regional divisions had ten, others eleven teams. It was obvious that in the latter case one team was necessarily idle each Sunday, but I wondered whether it would be possible to have not more than one team idle each Sunday in the divisions comprising an odd number of teams, and none idle in the even-numbered divisions. I solved the problem graphically, by placing the teams' names on the vertices of a polygon (cf. Figure 4, where the teams are named A,B,C,...etc.). Surprisingly, the problem turned out to be easier for the odd than for the even number of teams. I drew a set of parallel lines connecting vertices, as in Figure 5, representing the matches on the first Sunday. [For N teams, N being odd, there would be $\frac{1}{2}(N-1)$ games]. For the next Sunday I rotated the configuration one place (Figure 6), and the next another, until I had rotated all

the way around the polygon; each Sunday one team would have been idle, so N Sundays would have passed, and $\frac{1}{2}N(N-1)$ games played. Since there are just that many connections between N items, and my algorithm had not duplicated any connections, I can be quite confident that I had exhaustively and optimally enumerated a complete competition schedule for a division comprising an odd number of teams.

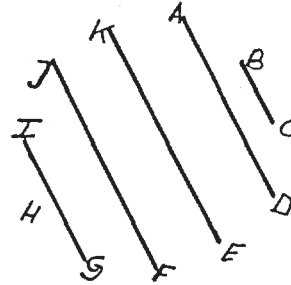
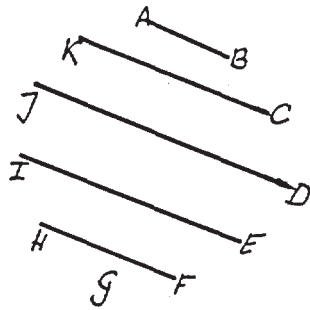


Figure 5: Eleven-team Competition, first Sunday

Figure 6: Eleven-team competition, second Sunday

As said, the method did not quite work for even numbers of teams. Figure 7 represents my example, showing ten teams. The first Sunday five games were played, according to the diagonals drawn in. However, it is evident that after $\frac{1}{2}N$ weeks, in each of which $\frac{1}{2}N$ games would have been played, the pattern repeats, so that the algorithm only generated $\frac{1}{2}N^2$ games. I noticed that my method only paired off teams that were an odd number of steps apart along the circumference of the polygon, whereas in the earlier example what was an even number of steps around the polygon in one sense, was an odd number in the opposite sense, so that, to mix a metaphor, all bases were covered. Accordingly, I had to add a configuration in which every team was matched with one an even number of places removed along the circumference of the polygon (Figure 8). This configuration left two teams idle, which in my case of ten teams were an odd number of places apart, hence did not need to be included. So this configuration yielded $\frac{1}{2}(N-2)$ games, and by rotation it could be used $\frac{1}{2}N$ weeks, yielding in total $\frac{1}{2}N(N-2)$ games. Combination of the two algorithms yields a total of $\frac{1}{2}N(N-1)$ games on N Sundays, and all was well.

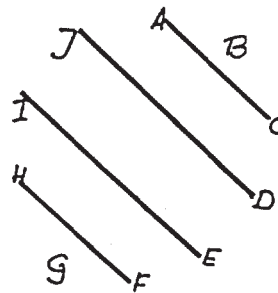
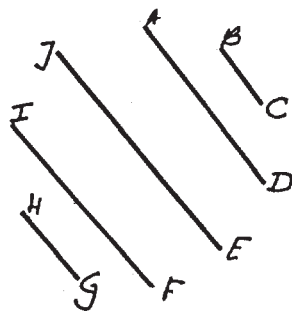


Figure 7: Ten-member competition, first Sunday
Figure 8: Ten-member competition, second configuration

Note that I had as a teenager dealt only with the particulars of ten-team and eleven-team divisions, not the general problem of N teams. After all, I was feeling rather guilty about taking time off from my homework assignment to play games without any apparent relevance to my schoolwork; moreover, my father, who had been an avid soccer player, and presently still follows the progress of his club, was rather mystified by my theoretical interest in soccer. It had never have occurred to me at the time to attempt a general algorithm, and it would never have occurred to me to return to this problem if it had not been for my former student, David Masunaga. David is a distinguished Mathematics teacher in Hawaii, who took a Master's degree at the Harvard School of Education a few years ago, and my course as part of his curriculum. The year after his graduation David returned to the class to conduct a workshop, and to my surprise brought in the soccer-competition problem. Just as Molière's M. Jourdain was amazed to discover that he had been speaking prose all his life, so I found out that my forbidden games had been mathematics all along. In point of fact, it is only now that I realize that the reason for keeping two teams idle when the division comprises an even number of teams is slightly different when that number is divisible by 4 from what it was in my example of ten teams. However, I leave that to the reader to determine: it is, in point of fact a matter of symmetry!

As a small child I had been given a board game comprising colored marbles and a playing board in which holes were located in a regularly spaced array, each hole being at the center of a regular hexagon at whose vertices were identical holes identically surrounded (Figure 9). The marbles were to be arranged in the holes to form certain patterns. I was given a booklet of patterns to copy on the board, but soon grew tired of this assignment, preferring to design my own patterns. Surprisingly, I was able to create rectangular, but not square patterns on the playing board. Unfortunately, this investigation turned into another forbidden game, for I was told to stick with the assigned patterns. The game remained suppressed for about thirty years, when, on the staff of MIT's Computer and Systems Group I tried to understand the structure of the mineral spinel, which is identical with that of the ceramic cores which we were designing for the memory of the Whirlwind computer.

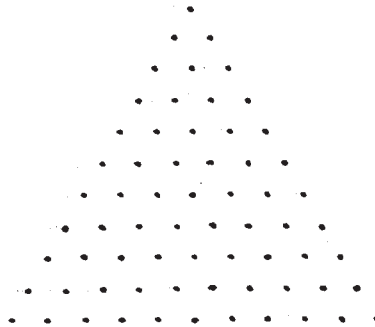


Figure 9: Hexagonal Array

I was not making much progress, and instead felt inclined to doodle: I wanted to subdivide the hexagonal net such that the subdivisions each formed a hexagonal array geometrically similar to the original; Figure 10a shows the subdivision into *three*, Figure 10b subdivision into *four* such sub-arrays. The question was whether the hexagonal array could be subdivided in this fashion into *any* number of sub-arrays. Certainly this appeared to be a forbidden game having no useful application when the sponsor is expecting to be enlightened about the spinel structure!

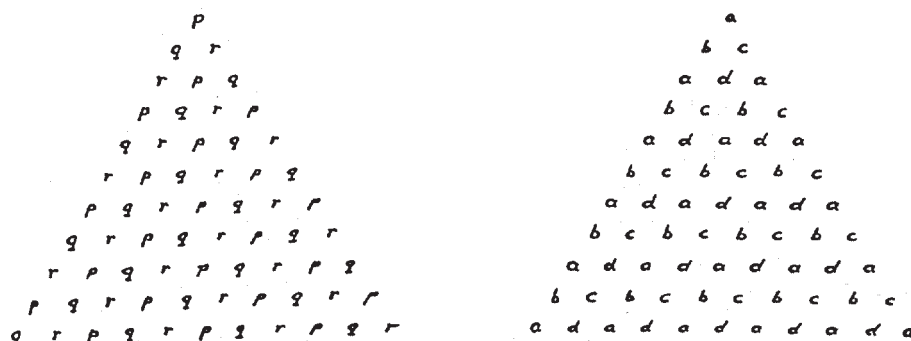


Figure 10a: Subdivision of the hexagonal net into three geometrically similar subarrays
 Figure 10b: Subdivision of the hexagonal net into four geometrically similar subarrays

Well, I was obsessed with my forbidden doodle, and found that the hexagonal net may be so subdivided into $k^2 + kl + l^2$ subarrays, where k and l are positive or negative integers or zero. The two examples of three and four subarrays correspond respectively to the combinations (1,1) and (2,0). The combination (2,-3) would lead to seven subarrays. More to the point, however, was that there are *no* values of the integers k and l which would make the expression $(k^2 + kl + l^2)$ equal to either 2 or 8. And, lo and behold, that gave me the clue to an understanding of the spinel structure (Loeb, 1964 and Loeb & Casale 1963)! Why the game of a five-year old should surface thirty years later to help solving a problem is beyond my understanding; this experience taught me, however, to trust my intuition, that un verbalized knowledge, a bit more, and to give more importance to the role of games.

As a result of the war, I never finished high school. I entered the University of Pennsylvania on the basis of College Board admission exams, and at age twenty was admitted to Harvard's Graduate School, which granted me a Ph.D. when I was twenty-five. No time for forbidden games any longer! After another five years I returned to the Netherlands for a year, and attended an international mathematical congress as a delegate for the Society for Industrial and Applied Mathematics. At that congress I saw for the first time the original works of M.C. Escher, of which I had only seen reproductions in Life magazine. In 1960 I met Escher at a meeting of the International Union of Crystallographers in Cambridge, England, and a close friendship developed (Loeb, 1982a,b).

Above I mentioned my grandfather's collection of Delft tiles, which is presently in the Rijksmuseum in Amsterdam. It is considered by some to be second only to the Loudon collection in the Prinsessehof in Leeuwarden in the north of the Netherlands. This museum was originally the residence of the stadholders of Friesland, the direct ancestors of the royal house of the Netherlands. In the garden of the museum is a small column, tiled with an Escher design, commemorating the fact that Escher was born in that palace when it had been subdivided into private residences. Indeed, tiles were part of our cultural heritage, and probably shaped our outlook.

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