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Stages in the construction of stereograms of molecular models

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In this article an analysis is performed of the results of stereogram construction using computer programs that model chemical compounds. Considerations about how best to represent models of molecules and improve legibility of stereograms are presented. An original diagrammatic substitute for the picture of a sphere, suitable for application in stereoscopic models of molecules, is proposed.

The number of visual means requiring a three-dimensional presentation of reality has been constantly increasing. Modern technology allows for fulfillment of many of those requirements, offering systems of recording and presenting dynamic spatial pictures.[1,2] However, as long as paper is the carrier of scientific information, the stereoscopic technique in its basic form will be used.[3,4] Because drawings used in publications mostly represent objects impossible to photograph,[5–7] an important role will be played by computer techniques for stereogram preparation, based on the theoretical assumptions of the mechanism of human perception of a spatial picture.[8]

Although the rules of perception of stereoscopic picture seem to be simple, it is possible to make many mistakes in making such a picture, and as a result to produce illegible stereograms. The objective of this article is to discuss the principles of construction of stereograms of the models of chemical molecules, using computer programs. The main aim is to present our considerations leading to identification of the best way of developing the models of molecules and to assure their faultless legibility.

Stereoscopy is not the only method of conveying information about depth.[9] On the basis of the analysis of the way a human perceives the world it is possible to identify a whole spectrum of both graphic and physiological effects that can be of help in presenting spatiality (Table 1). Application of many of the effects may effectively increase the legibility of the picture of models. Their importance depends on the specific character of the observed object.

Color Plates for this article are on page 94.

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Table 1. Types of identified effects

Physiological	Accommodation
	Convergence
Geometric	Stereopsis
	Linear perspective
	Static interposition
Psychological	Size stability
	Shape stability
	Light and shade
Kinetic	Kinetic interposition
	Kinetic parallax
Aerial	Aerial perspective
	Texture gradation
	Tarnishing-color

In essence, the idea of stereoscopy is simple. It is based on the observation that the human left eye sees a different image than the image perceived by the right eye. The differences are the result of the positions of the eyes, i.e., there is a difference between the viewpoints of observation of the same object. Hence it is possible to determine the rules according to which any picture can be mathematically transformed so as to prepare images perceived by each of the eyes.[10]

One can easily suppose that to obtain an image perceived by one eye, we can apply either a nonorthogonal projection on the plane or an orthogonal projection of a rotated object (Figure 1). The latter is the more tempting in that if often turns out to be more simple, especially via computer programs producing pictures of models, to transform the picture via rotation rather than via projection. Application of rotation, however, often leads to distortions of the stereoscopic picture,[11] as it involves rotation of the plane onto which the picture is projected. Hence, such a picture should be viewed only after it is placed on the cylinder wall, which is not accepted in the convention of stereogram presentation.

Construction of a correct algorithm of projection of an object's picture on a plane does not solve the problem of the correctness of imaging. Many programs for stereogram construction prove useless if they do not take into account the

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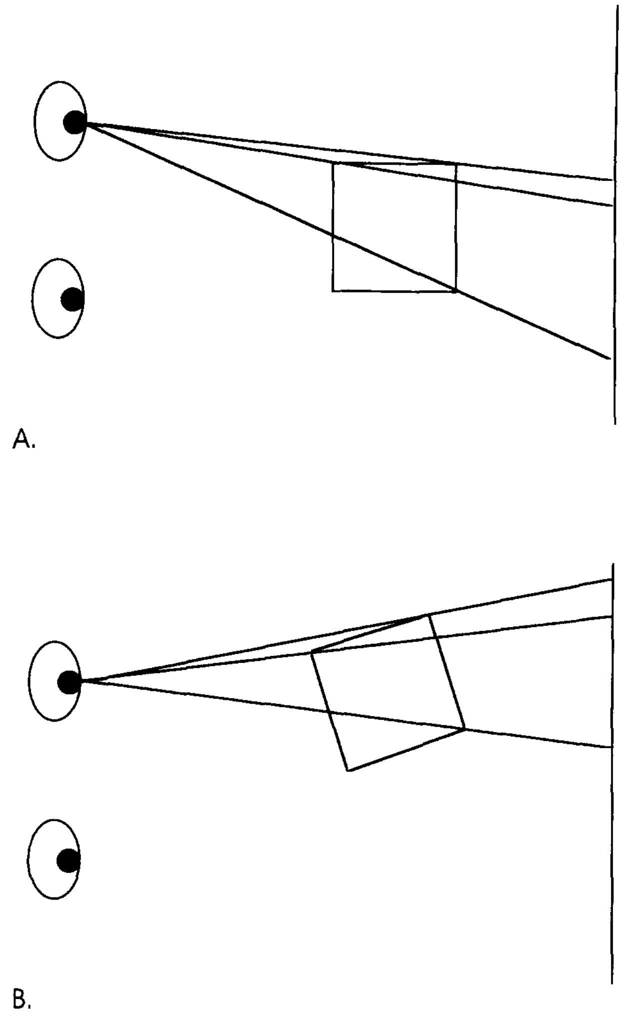

Figure 1. Models of imaging for stereoscopic recording. (A) Nonorthogonal projection on a plane; (B) orthogonal projection of a rotated object.

perspective (as a geometrical consequence of perception) of a picture of an object by a significantly smaller object, i.e., an eye. Perspective must be accounted for in the calculations of projection both for the whole perceived object and for each of its elements. In the first place it should be considered in calculating the size of the pictures of spheres symbolizing atoms in the drawing of a model of a chemical compound.

Hiding of objects that are more distant from the observer by closer lying objects, also called static interposition, may provide the basis for determining the spatial relations of the model. This does not have to be taken into account in the case of the presentation of dynamic pictures of models, yet it should be remembered in the case of stereoscopic drawing. By picturing the rotated object in such a way that the selected atoms partially overlap, it is possible to improve the legibility of the spatiality of the model.

For models of chemical compounds, of paramount importance is the ability of a person—related to the effect of linear perspective—to discern the depth of the picture on the basis of the stability of size. In many situations this effect permits proper spatial location of objects of the model. Such a situation is illustrated by the model of a tetrahedral molecule shown in Color Plate 1. The light spheres seem to present atoms of the same type, thus of the same size. In the drawing their sizes differ, since spheres placed further from the observer are presented as smaller.

For presenting pictures of large crystalline structures, it is important to consider the possibility of applying the effect of shape instability. In such cases an impression is evoked that with increasing distance from the observer the sharpness of a picture of a body decreases, as well as its angles—thus a square resembles a circle. This effect can occur only in models comprising nonoval objects, i.e., tetrahedra.

In constructing pictures of spatial models, the application of the light–shade effect must also be considered.[12] Although shading is not a natural way of creating depth perception, it is often used as an aiding factor in the methods for presenting spatiality. We should distinguish three aspects of light–shade effect production (Figure 2):

1. The first type, often applied, concerns generation of shades by an object on itself. This effect is popular because it may be applied as the only expression of depth of the presented object.[13]
2. The second type consists of shades generated by the pictured object on neighboring objects. Limited application of this type results from the fact that it may decrease the legibility of the picture.
3. The third type includes shades generated by the pictured model on the ground where the object is placed. This type cannot be applied in pictures of models of chemical compounds, since the tendency is to avoid showing the ground so as to emphasize the features of space in which atoms are placed.

The applicability of the first of the aforementioned effects is the greatest, however it can not be considered for the stereoscopic pictures. As has already been mentioned, shade generation is a feature of space perceived by an observer owing only to his or her previous experience and knowledge, and is not due to elementary brain analysis.

The effects of shade generation should be clearly distinguished from the effects of light reflection on the surface of an object. A programmer is tempted to account for the reflections, yet in the case of stereograms their application may result in many deviations. Most of them may result from the fact that changes in the angle of reflected light are proportional to changes in the angle of incident light. As a consequence, the dependencies of the reflections perceived by each eye are reversed relative to the dependencies of the observed object and shade elements. A good illustration of the above is to look at stereoscopic pictures of a steel sphere or a teaspoon, and attempt to indicate which of the images is perceived by the left and which by the right eye.

Likewise, the light–shade effect may lead to the effects classified as defects of ''binocular depth inversion''; convex objects may—due to light arrangement—seem to be concave.[14] In the case of models of spheres, even application of interposition, which usually levels out the effect of inversion, does not bring satisfactory results. Besides, it should also be remembered that the aim of making the picture of a model is to print it on paper, which often implies reduction of the coloring spectrum to two colors: black and white. Application of the techniques of color reduction (such as the raster method and the dithering method), in-

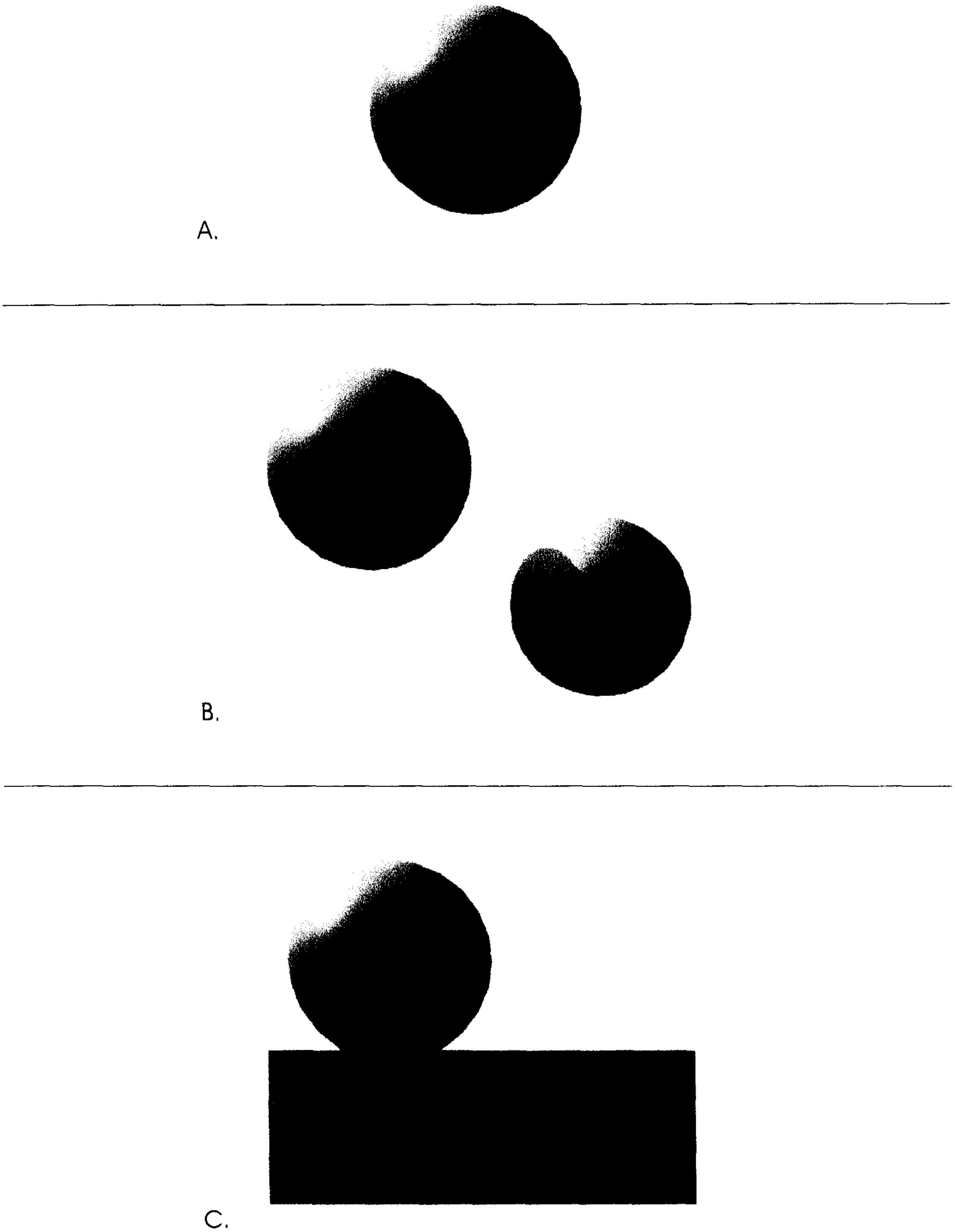

Figure 2. Three aspects of light–shade generation: (A) production of shades by object on itself; (B) production of shades by the pictured object on neighboring object; (C) production of shades by the pictured model on the ground where the object is placed.

stead of improving the legibility of stereograms, intensifies the problem of perception. To understand the reasons for such distortions we should analyze the conditions of binocular vision.

The concept of spatiality is generated by the mind because of the differences in the compositions of two images; the more pronounced the differences, the more easy it is to perceive the depth. Hence it is not surprising that it is easier to define spatiality of simple rather than complex objects, provided the number of comparable elements is sufficient. Spatiality of a solid (e.g., a TV set) is defined by comparing the object to an elementary cuboid. By analogy, spatiality of a sphere is defined by comparing it with a circle. Yet a circle is planar—and this is why in a stereoscopic picture it is

```
program ellipse;
var
i, centr_x, centr_y, radius : Integer; x, y, z, gamma, delta, alpha : real;

begin
 centr_x := 255;
 centr_y := 135;
 radius := 135;
 gamma := (20 + 90) / 180 * pi;
 delta := (20 + 90) / 180 * pi;

{starting point}
 alpha := 0;
 x := radius * cos(alpha);
 y := 0;
 z := radius * sin(alpha);
moveto(trunc(x * sin(gamma) + (z * sin(delta) - y * cos(delta)) * cos(gamma) + centr_x),
trunc(y * sin(delta) + z * cos(delta) + centr_y));

{following points}
  for i := 1 to 360 do
   begin
   alpha := (i * 1 / 180 * pi);
   x := radius * cos(alpha);
   y := 0;
   z := radius * sin(alpha);
   lineto(trunc(x * sin(gamma) + (z * sin(delta) - y * cos(delta)) * cos(gamma) + centr_x),
    trunc(y * sin(delta) + z * cos(delta) + centr_y));
   moveto(trunc(x * sin(gamma) + (z * sin(delta) - y * cos(delta)) * cos(gamma) + centr_x),
    trunc(y * sin(delta) + z * cos(delta) + centr_y));
   end;
end.
```

Figure 3. A mathematical calculation of ellipse that accounts for spatial rotations.

perceived as a planar object, irrespective of the algorithm of shading. To be even more accurate, the picture of a shaded sphere is perceived in a simplified form as a system of two circles: a light circle and a dark one.

For the picture of a sphere to be perceived in stereoscopy, it is necessary to replace the whole description of a sphere by its symbolic, or schematic, substituent.[15] This substituent should have distinguishable, spatial elements that in each geometrical projection would behave differently, thus being liable to comparison. A number of those elements should depend on the degree of complexity of the structure of the modeled molecule. It is easy to conclude that if the number of atoms in a molecule exceeds 10, then in the picture of such a model the relations between atoms are more pronounced than are the relations within each atom. Only when the number of intramolecular correspondences is lower does the problem of "planar spheres" become apparent.

The substituents of the picture of a sphere should be universal. Its spatial elements that are to be compared should not be numerous, thus assuring the most faithful imitation of spheres, and they regularly should take new shapes on geometrical transformation. Computer programs are not based on a diversified set of substituents. The most popular of them do not seem to be legible enough (models

A–D; Color Plate 2). The present authors suggest application of an object made of parallel circles nine by three, perpendicular to the axis of the coordinate system that seems to satisfy best the above-mentioned requirements (model E; Color Plate 2). Naturally, it seems important to illustrate the rotated model, to emphasize the differences in the drawing of characteristic elements. It is important to remember that the change in shape of a circle on a multifunctional rotation does lead to a pure ellipse, and therefore such a simplification should never be taken into account.

Figure 3 is a mathematical calculation of ellipse that accounts for spatial rotations.

Marginal, although not absent elements of the perception of depth are the effects related to aerial perspectives—gradation of surface quality, tarnishing, and changes of color. Each of these elements is capable of recording information about depth, yet they are of advantage only for presenting pictures of large crystalline structures or macromolecules, to emphasize their sizes.

There is no need to present a thorough discussion of the features of a system of two stereoscopic drawings. A proper selection of the distance between the drawings, selection of the recommended distance between the eyes of the viewer and the picture, and the assumed spacing of eyes to a large degree determine the legibility of stereoscopic pictures.

In the case of chromostereograms a proper selection of colors is also of importance. It is possible to apply one of the three color combinations: red–blue, red–green, and blue–green, with the sequence of color application being insignificant. Analysis of the intensity of perception of particular basic colors and the analysis of contrasts of the above systems suggest that only two systems are optimal as regards the application of stereoscopic pictures: the red–blue and red–green.

A detailed investigation of different elements of perception of a spatial picture permits determination of significant features in the drawing of a stereoscopic model of a molecules and thus to avoid making mistakes in picturing the model. Compliance to the rules resulting from the above can even contribute to increasing the legibility of stereograms. Many of the discussed issues can be applied in the techniques of stereoscopic picture generation using computer programs.

All of the above considerations do not apply to stereoscopic pictures recorded using synchronized cameras or similar techniques of recording pictures and analogous methods of presentation of a spatial picture.[16–18] Also, for obvious reasons, considerations of the physiological and kinetic effects of the description of object spatiality have been omitted.

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