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Crystallographic autostereograms

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Perspective drawings of crystal structures can be presented as autostereograms (or single-image stereograms), and their performance for in-depth perception is similar or even more advantageous than of stereopairs. The autostereograms offer a convenient means for realistic insight into crystal structures without excessive size reduction of their drawings, as required when preparing stereopairs; thus structures either as simple as elements or as complex as proteins can be illustrated in enhanced resolution. The mathematical background and guidelines for preparing crystallographic autostereograms are described. © 2001 by Elsevier Science Inc.

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INTRODUCTION

Three-dimensional perception of crystal structures is a vital element of scientific research, of passing information and understanding complex geometrical problems, while presentations of scientific results are naturally limited to two dimensions of the paper or screen surface. Therefore stereoscopic pairs are applied frequently in crystallographic, physical, chemical, or biological publications where structure–property relations are analyzed. The concept of a stereoscope, invented in 1838 by C. Wheatstone[1,2] and improved by D. Brewster by utilizing lenses, was presumably first applied in a crystallographic public-domain computer program, *ORTEP*, in 1965 by C.K. Johnson,[3] and is now widely used in many variations (anaglyphs, shutter eyewear, etc.). The method most commonly used in scientific publications is the presentation of a stereopair: two drawings of an object, a molecule, or crystal structure, with one rotated with respect to the other by approximately 6° about the vertical axis, the angle corresponding to the difference in the viewing angle of human eyes. The drawings are placed side by side, with the distance of about 6 cm between their equivalent points. This latter condition restricts the size of the drawings, and hampers their use without special glasses; the decreased resolution of small drawings also limits the number of fine details that may be included and distinguished. Meanwhile, growing interest in molecular association, weak interactions, long-range structural correlations, as well as increasingly complex structures tackled crystallographically, particularly in the fields of supramolecular and biological chemistry, requires that larger portions of crystal structures be presented, for which traditional stereopairs are inadequate. New methods of efficient stereoscopic presentations are clearly needed. Moreover, the advent of area detectors, particularly of CCD cameras, has dramatically increased the number of structural determinations. A plenitude of structures are often processed routinely and dumped to databases, while efficient methods of rendering crystal structures could facilitate their more scrupulous analysis.

This article shows that perspective drawings or photographs of periodic objects contain the information equivalent to those in stereopairs. When a perspective drawing of a crystal structure is prepared according to the recommended guidelines, it can be easily perceived in three dimensions and is ideal for black-and-white or color presentations of crystal structures or molecular aggregates.

METHODOLOGY

Depth perception is produced when an observer's two eyes focus and converge on an object at somewhat different angles (Figure 1). The mathematical formula for the angular difference, δ, at which a small object, O, is viewed depends only on the coordinates of the object, (x^o, y^o), and of the eyes, (x_1^e, y_1^e), (x_2^e, y_2^e):

$$\delta = \tan^{-1}\left(\frac{x^o - x_2^e}{y^o - y_2^e}\right) - \tan^{-1}\left(\frac{x^o - x_1^e}{y^o - y_1^e}\right). \qquad (1)$$

This angular difference can be also expressed in the terms of separation between the eyes, d, and of distance b from the object to axis **y**:

$$\delta(b, d, y) = \tan^{-1}\left(\frac{2b + d}{2y}\right) - \tan^{-1}\left(\frac{2b - d}{2y}\right), \qquad (2)$$

by making the following substitutions in Equation 1: $x_1^e = -d/2$, $x_2^e = d/2$, $y_1^e = y_2^e = 0$, $x^o = b$, and $y^o = y$. The direction of vector **d** will be also referred to as the horizontal direction later in this paper, and angle δ as a rotation about the vertical direction. Equations 1 and 2 can be applied for calcu-

Color Plates for this article are on page 398.

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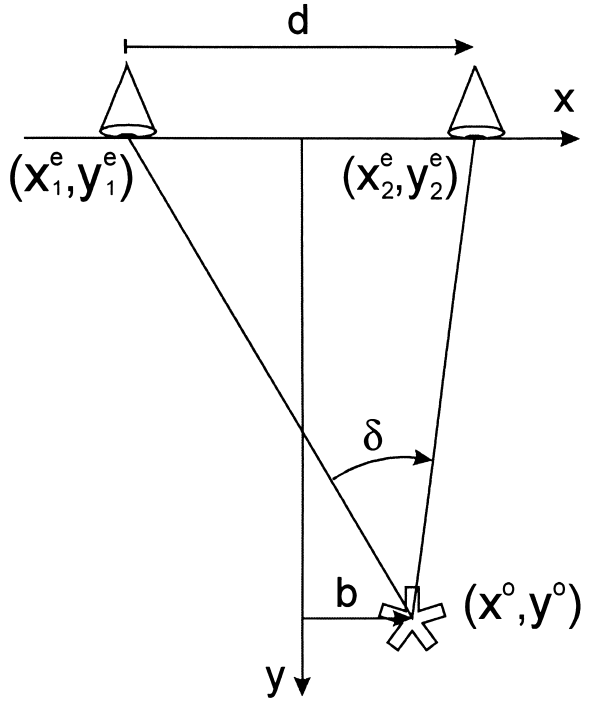

Figure 1. Small object O *viewed from two points separated by distance d along axis* **x***; δ denotes the angular difference in the viewing the object. Angle δ is ~6° for the objects seen from ~50 cm, but in this and in subsequent schemes it has been enhanced for clarity.*

lating the angular difference in viewing any element of a complex object. However, when a complex object comprises several translationally identical elements, as shown in Figure 2, a general formula for the angular difference in viewing the *n*-th element can be derived:

$$\delta_n = \tan^{-1}\left(\frac{2na + 2b_o + d}{2y}\right) - \tan^{-1}\left(\frac{2na + 2b_o - d}{2y}\right), \tag{3}$$

where b_o is the distance from axis **y** to the closest element, labelled $\mathbf{O}_0$, and vector **a** represents the translational symmetry of the pattern; for simplicity it is assumed that **a** is parallel to axis **x**. Thus, δ_o denotes the angular difference in viewing element $\mathbf{O}_0$ from two points separated by d, δ_1 is the angular difference in viewing element $\mathbf{O}_1$, etc. When the periodic object is viewed from one point, at (x^e, y^e), the translationally related elements of the pattern are seen from different angles, too, as shown in Figure 3. The general formula for the angular difference in viewing neighboring elements n and $(n + 1)$ is:

$$\delta_{n,n+1} = \tan^{-1}\left(\frac{x_{n+1}{}^o - x^e}{y_{n+1}{}^o - y^e}\right) - \tan^{-1}\left(\frac{x_n{}^o - x^e}{y_n{}^o - y^e}\right), \tag{4}$$

where (x_i, y_i) are the coordinates of i-th element of the pattern. By substituting $x_n{}^o = na + b$, $x^e = 0$, $y^e = 0$, and $y_n{}^o = y$ for all $n = 0, \pm 1, \ldots$ this equation can be rewritten in terms of the translation a and offset b:

$$\delta_{n,n+1} = \tan^{-1}\left(\frac{(n + 1)a + b}{y}\right) - \tan^{-1}\left(\frac{na + b}{y}\right). \tag{5}$$

By further assuming $b = b_o - d/2$ and $a = d$, Equation 5 for $\delta_{n,n+1}$ becomes identical with Equation 3 for the angular difference in viewing one element from two points:

$$\delta_{n,n+1} = \tan^{-1}\left(\frac{2na + 2b_o + d}{2y}\right) - \tan^{-1}\left(\frac{2na + 2b_o - d}{2y}\right). \tag{6}$$

The y-coordinate of such a translationally symmetrical object is constant and equal to the object–eye (camera objective) distance, l. Thus, Equations 3 and 8 differ only by the difference between $d/2l$ and $a/2l$, as well as between b and b_o. The difference between these values for the pictures where vector **a** is parallel to **d** may be close to zero, or may be adjusted to be small when preparing and scaling the drawing.

The similarity of Equations 3 and 5 implies that for periodic objects the information about their three-dimensional nature is contained in their perspective picture, even though it is recorded from one point, as shown in Figure 3. This information is encoded faithfully in the single image in the same manner, as if each element were viewed by two eyes. Thus, a perspective picture of a periodic object can be perceived three dimensionally when the eyes are converge to see neighboring elements: eye *1* on element *n* and eye *2* on element $(n - 1)$. Then the elements and their arrangement are perceived in three dimensions identically, as if they were viewed by two eyes.

The method of encoding three-dimensional images into distortions of translationally symmetrical patterns and then decoding them by misleading eye convergence has long been used for artistic expression and in children books (often called *Magic Pictures*, etc.), and such pictures are usually called single image stereograms (SIS), autostereograms, or single image random dot stereograms (SIRDS). Although the principle of encoding the third dimension in such pictures is different than in perspective pictures of crystal structures described above, the method of perceiving the third dimension in both cases is similar: by converging and focusing eyes on the neighboring elements of the patterns. Hence, such perspective images of crystal structures can be referred to as crystallographic autostereograms or crystallographic single-image stereograms.

The physical meaning of the sign of δ in Equations 4–6 is that the stereopairs have to be viewed by diverged eyes, whereas the autostereograms should be viewed by converged eyes. The sign of δ may be arbitrarily assigned as positive for converged, and negative for diverged eyes. Viewing the stereopairs or autostereograms can be aided with appropriate special glasses. However, it is a more natural function to converge than diverging, and autostereograms can be conveniently viewed without the glasses. In practice, stereoscopic pairs are often viewed without glasses by converging eyes, too. These images also produce depth perception, but the third dimension is inverted perpendicular to the drawing.

As the autostereograms consist of one drawing, its viewing orientation may be not always immediately obvious. Therefore, the translational symmetry should be embedded horizontally in the text. Diagrams of crystal structures may contain several translations, and different perspectives of viewing the same

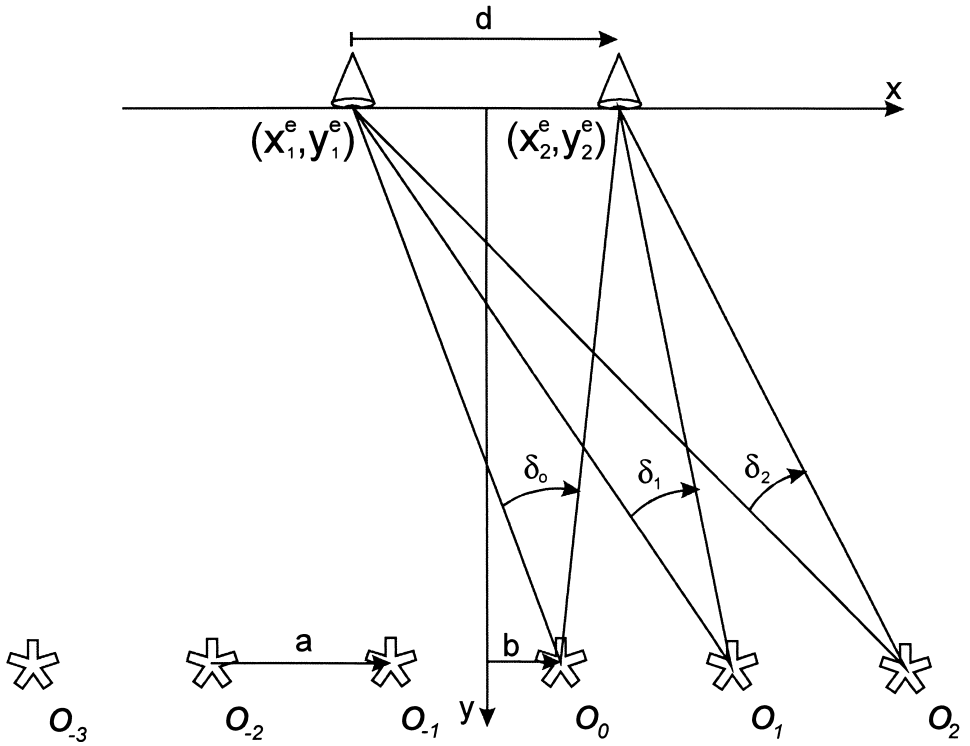

Figure 2. A periodic object viewed from two points: the vector of translational symmetry, **a***, is parallel to* **x** *and* **d***, and relates the neighboring elements; vector* **b** *measures the displacement of the element labelled* $\mathbf{O}_0$ *closest to axis* **y**.

autostereogram can then be obtained by orienting the required translation horizontally (i.e., parallel to the eyes' line), provided that the translations are at least approximately parallel to the surface of the drawing. The translational symmetries of the crystal structure may be conveniently indicated by including the unit-cell into the autostereogram. It should be noted that the impression of three dimensionality of the unit cell mainly derives from its skew lines superimposed by the vergence of eyes. Therefore one should avoid superimposing front and rear edges when drawing a crystallographic unit cell, while it is advantageous that the front and rear edges are equally spaced on the left and right side of the unit cell.

DISCUSSION

Autostereograms offer a convenient means of presenting crystallographic data. Ther are several advantages of the autostereograms: (i) autostereograms can serve as a normal perspective illustration of crystal structure (and conversely, many perspective drawings already published may be viewed as autostereograms in three dimensions); (ii) the "typical" autostereogram contained in the 8-cm column of a journal article is approximately two times larger than each drawing of a stereopair, thus more details can be included; (iii) there are no limits to the size of the autostereogram, which may cover a full page of a journal; (iv) autostereograms are more accessible for the readers because it is a more natural function of eyes to converge rather than diverge. Most students presented with autostereograms for the first time perceive them in three dimensions after few moments, much quicker than stereopairs even with help of special glasses. The disadvantage of autostereograms is that only the portion of the pattern including *n* translations, superimposed with itself after applying the translation (by converging the eyes) can be perceived three dimensionally. Thus, the perceived picture will contain $(n + 1)$ elements, $(n - 1)$ of them three-dimensional, and two terminal, left and right ones, which are flat. Like other methods of stereoscopic presentations, autostereograms are equally well suited for printed or animated pictures, when the elements synchronously move or transform, although animated rotations of the whole object may be executed only about the horizontal direction. Naturally, the translational symmetry is the necessary condition for creating autostereograms; therefore, asymmetric molecular fragments or molecules cannot be presented in this way.

The example of the autostereogram in Figure 4 shows the crystal structure of the monoclinic polymorph of maleic hydrazide.[4] This crystal is built of the maleic hydrazide molecules hydrogen bonded into double chains along **x**. The autostereogram contains several translations, and can be viewed with these vectors oriented horizontally. Three such translational repetitions are shown along axis **x** and this direction is most convenient for viewing the structure. When the eyes are converged on neighboring molecules (the OH—O bonded ones) the emerging picture contains two unit cells side by side along **x**, and four molecules in each chain, the central two of which result from superposition of neighboring elements and are perceived in three dimensions. This picture gives a clear impression of the arrangement of the neighboring overlapping chains, and of the fine crease along the hydrogen-bonded supramolecular ribbons. This autostereogram can be also viewed after rotation by 90°, so the elements translationally related along **y** are superimposed. In this case a complete three-dimensional view of two central chains is obtained. As explained above, the rotation of the autostereogram changes the portion of the drawing that is perceived in three dimensions. The example in Figure 4 also illustrates the usual property of most crystals, that the

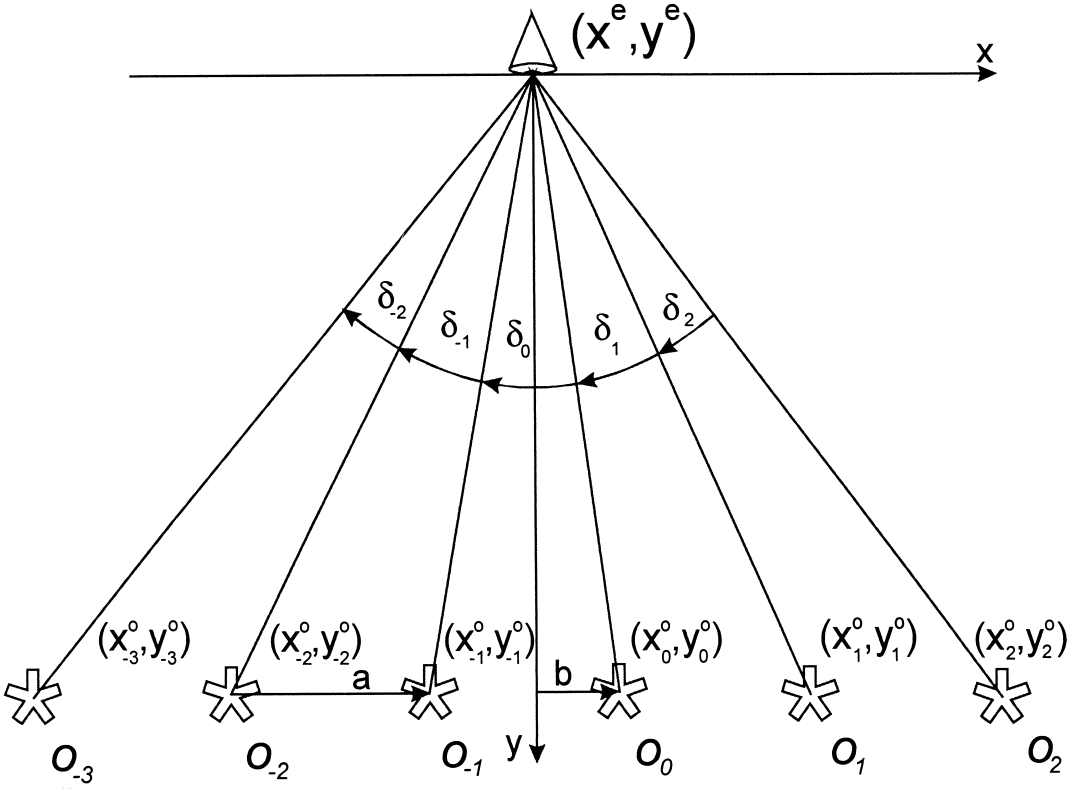

Figure 3. Periodic object composed of multiple translationally related elements viewed from one point.

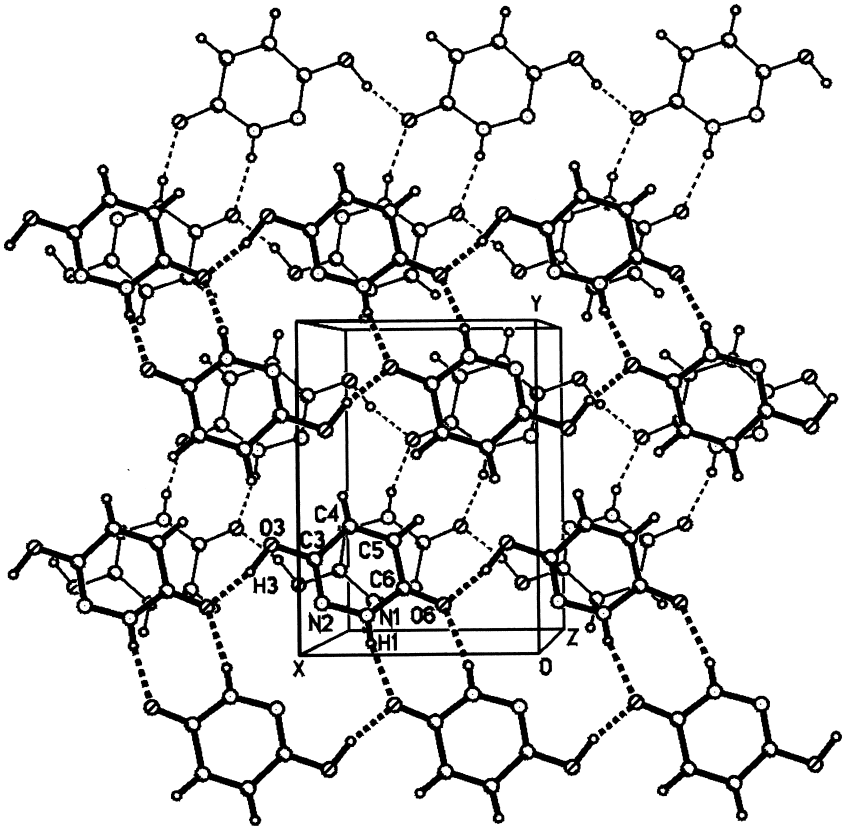

Figure 4. Autostereogram of the monoclinic polymorph of maleic hydrazide[4]: the hydrogen bonds have been indicated by dashed lines, while thick and thin lines have been used to discriminate between two layers of the molecules down **x**.

shortest dimension of the unit cell coincides with the strongest interactions forming the supramolecular aggregates, parallel to **z** in this figure. Incidentally, this feature is beneficial when preparing autostereograms of crystal structures and supramolecular aggregates, as the short horizontal translation allows the size of the drawing to be maximized.

Naturally, the inclusion of the unit cell is not necessary: the next example in Color plate 1 shows a helix of hydrogen-bonded cations in the crystal of N(1)-oxide-17-oxosparteinium perchlorate.[5] The crystal is monoclinic, space group $P2_1$, and cations of three symmetry-independent ionic pairs form one turn of the helix running along **z**, while the ClO_4^- anions are located outside the helix in the gaps between the helices in the crystal. In this autostereogram the translational symmetry is horizontal and only in this direction can the helix be viewed stereoscopically.

Figure 6 shows 5 × 5.5 unit cells of 1,4-diazabicyclo[2.2.2]octane perchlorate, the first ferroelectric for which transition to the paraelectric phase involves disordering of protons in NH— —N hydrogen bonds.[6] This example shows that the overall size of autostereograms is not limited and, apart from larger and clearer illustrations, they may be also applied, for example, for designing posters or book covers.

The examples presented above have been prepared with program XP of Siemens.[7]. It is expedient that the autostereograms can be generated using software which is already in use—most commonly available programs, such as *ORTEP*[3] or *PLUTO*,[8] can draw perspective pictures of crystal structures. However, it should be noted that most programs for protein graphics may produce only projections of structures (also applied by these programs for generating stereopairs by shear rotations), and as these programs cannot draw perspective views, they cannot be used for making autostereograms either.

CONCLUSIONS

Perspective two-dimensional pictures of translationally symmetric objects contain most information necessary for reconstructing their third dimension, and the brain's natural function of superimposing views from two eyes may be conveniently employed for depth perception of autostereograms similarly as it is done for stereopairs. Autostereograms offer an alternative to stereopairs for analyzing three-dimensional structures and their presentations in scientific publications. Autostereograms appear particularly suited for crystallographic presentations, as translational symmetry is intrinsic to crystals. The main advantages of autostereograms are their double function, either as normal perspective drawings or autostereograms, no requirement for excessive size reduction of the elements nor of the overall size of the picture, the possibility to view one drawing at various angles that somewhat changes the perspective, and finally no necessity of special viewers, as for anaglyphs or stereograms. We hope that the methodology of the autostereograms[9] will facilitate the clear presentation and analysis of crystal data, and that it will prompt further studies on presentations of three-dimensional geometrical and structural problems.[10,11]

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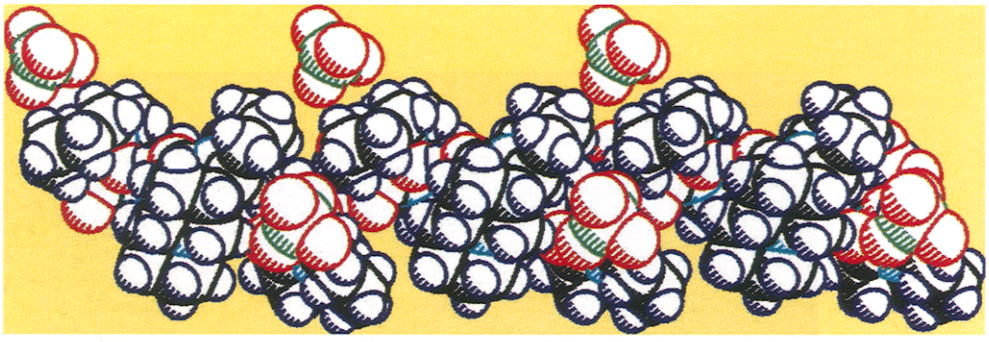
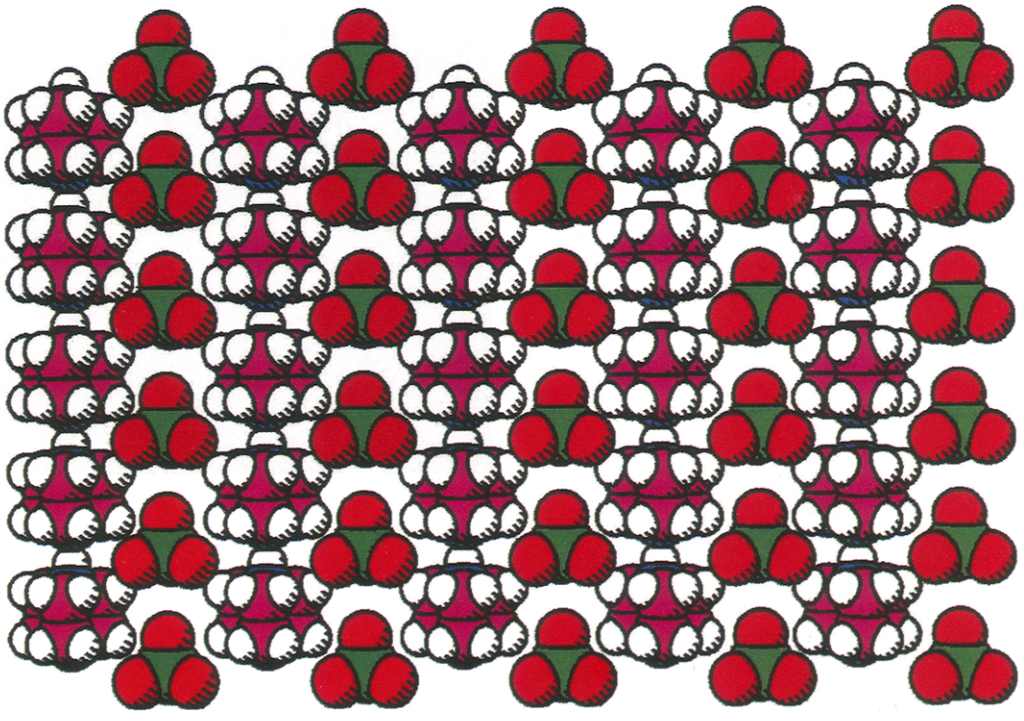
Crystallographic autostereograms



Color Plate 1. Space-filling autostereogram of one helix of hydrogen-bonded cations and anions in the crystals of N(1)-oxide-17-oxidespartein-ium perchlorate[5].



Color Plate 2. Space-filling color autostereogram of 5 × 5.5 unit cells of 1,4-diaza-bicyclo-[2.2.2]octane perchlorate vied down [y], [x] is horizontal and [z] vertical. Like Figure 4, this autostereogram can be viewed horizontally and vertically.