

ATLAS OF OPTICAL TRANSFORMS

G. Harburn, B.Sc.(Tech), Ph.D.

C. A. Taylor, B.Sc., Ph.D., D.Sc., F.Inst.P.
and

T. R. Welberry, M.A., Ph.D.

University College, Cardiff

Cornell University Press
Ithaca, New York

Copyright © 1975 by
G. BELL & SONS LTD
Portugal Street, London, WC2A 2HL

First published 1975

All rights reserved. Except for brief quotations in a review, this book,
or parts thereof, must not be reproduced in any form without per-
mission in writing from the publisher. For information address Cornell
University Press, 124 Roberts Place, Ithaca, New York 14850.

First published 1975 by Cornell University Press

International Standard Book Number 0-8014-0986-1

Library of Congress Catalog Card Number 75-14718

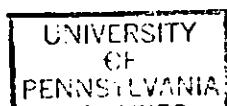
MATH-PHYS

QD

945

H37

Printed in Great Britain



Contents

Introduction—English	1
—French	3
The Plates	
1. Simple shapes and spacings	
2. Superimposed fringes	
3. Two hexagons	
4. Combination of hexagonal arrangements	
5. Addition	
6. The effect of orientation	
7. Orientation	
8. Symmetry operations	
9. The contribution of atoms in a unit cell to a particular X-ray reflection	
10. Development of a lattice	
11. Lattices	
12. Diffraction by a crystal	
13. Convolution and multiplication	
14. Circular and spiral lattices	
15. Perfect and paracrystalline lattices	
16. Gas and powder patterns	
17. General disorder	
18. Short-range order	
19. Stacking faults	
20. Thermally disturbed lattices	
21. Diffraction effects from fibres. I	
22. Diffraction effects from fibres. II	
23. Helices	
24. Coiled coils and double helices	
25. Small-angle scattering	
26. Diffraction effects of a gauze	
27. Phase control with mica	
28. Non-central sections of three-dimensional transforms	
29. Optical Fourier synthesis	
30. Spatial filtering	
31. Spatial filtering	
32. Spatial filtering	
Appendix 1 Apparatus and Techniques	5
Appendice 1 Appareils et techniques	9
Appendix 2 Notes on the plates	13
Appendice 2 Notes sur les planches	22
Appendix 3 Bibliography	32

Introduction

The idea of using optical analogues to aid in the interpretation of X-ray diffraction patterns originated with Sir Lawrence Bragg round about 1938, and it has been developed in many directions in the following thirty-five years. Most of the developments have been attempts to use the techniques to solve particular research problems and many have been successful to a greater or lesser extent. One common thread is apparent in the writings of all those who have published papers on the subject—the great power of visual presentation in teaching, in stimulating thought and in aiding the development of intuition, which still plays a major role in solving the more complex diffraction problems. The apparatus required for preparing optical diffraction patterns may be as simple as a remote lamp viewed through a photographically reduced mask representing the trial object, or a highly sophisticated system of laser and lenses capable of recording diffraction patterns from objects consisting of large holes punched in card. Discussion about the experimental needs for different applications still goes on, but a second thread common to many recent discussions has been that a generally available ‘Atlas’ of diffraction patterns (or optical transforms as they have come to be called) would be of great value.

A few years ago the Commission on Crystallographic Teaching of the International Union of Crystallography set up a pilot publishing programme with financial support from UNESCO and the Atlas project seemed a suitable item for this scheme. Unfortunately—or possibly fortunately in the event—the initiation of this programme coincided with a period of rapid development of optical diffraction techniques and the all too common dilemma of choosing between a poorer quality, but more or less immediate, publication or much improved quality with some delay, had to be faced. The delay has proved to be longer than we had hoped, but we feel that it has been worthwhile because of the higher standard of the diffraction patterns and the greater range of objects that eventually have been included.

We have tried to plan the Atlas so that it can be used for a wide range of purposes and the text has been deliberately kept to a minimum so that teachers may use the material in the way most suited to the needs of their students. It seems clear that it could be used in courses on optics, image processing, electron microscopy, astronomy and many other topics in addition to the interpretation of X-ray diffraction patterns which provided the original motivation. It should prove useful whenever visual presentation of Fourier transforms as two-dimensional photographs would be an advantage.

Technical details of the instruments and procedures used both in making the masks and preparing the diffraction patterns are given in Appendix 1. Appendix 2 consists of brief notes on the ideas underlying each plate. References are listed in Appendix 3, which includes a short bibliography of related publications.

ATLAS OF OPTICAL TRANSFORMS

Each plate consists of two blocks of twelve photographs which are numbered as follows for ease of identification.

1	2	3
4	5	6
7	8	9
10	11	12

With the exceptions of Plates 30-32 the diffracting objects are represented on the left-hand page and the corresponding diffraction patterns are on the right-hand page. Where the complete object is shown it appears as black on white, but for those objects in which the detail is very small only an enlarged portion of the mask is shown and, with a few obvious exceptions, these appear as white on black. All the diffraction patterns are white on black.

To help the reader relate features of the patterns to distances in the diffracting objects the plates have scales marked on them. The distance between adjacent scale marks for the diffraction patterns is reciprocally related to the separation of adjacent marks on the object plate. In other words, if a pair of holes of spacing equal to the separation of adjacent scale marks on the mask page were used as an object then, with the particular instrument and enlargement used, the resulting Young's fringes would have a spacing equal to the separation of adjacent scale marks on the transform page. Plate 1, No. 2, illustrates this point exactly. In a few cases the scale changes within a page. The scale marks are then shown on an individual photograph and apply to that and subsequent photographs in the sequence unless a new scale is shown.

Appendix 1

Apparatus and Techniques

A OPTICAL EQUIPMENT

A very small number of the diffraction patterns shown in this Atlas have been prepared on an optical diffractometer of the type described by Taylor and Lipson (1964). The main features of such a diffractometer are shown in Fig. 1. The source S_0 is a high-pressure, mercury-vapour lamp the arc of which is imaged by the condenser lens L_0 on to a pinhole which provides a secondary source at S_1 . The pinhole is in the back focal plane of a collimating lens L_1 , and is imaged in the focal plane F of the objective lens L_2 . The Fraunhofer diffraction pattern of a mask M , placed in the parallel portion of the beam, appears at F where it may be photographed or viewed with the help of a microscope.

The main disadvantage of the instrument is the low level of illumination in the diffraction patterns produced on it. The low intensity results from ensuring adequate temporal coherence by using a narrow band interference filter and creating the necessary spatial

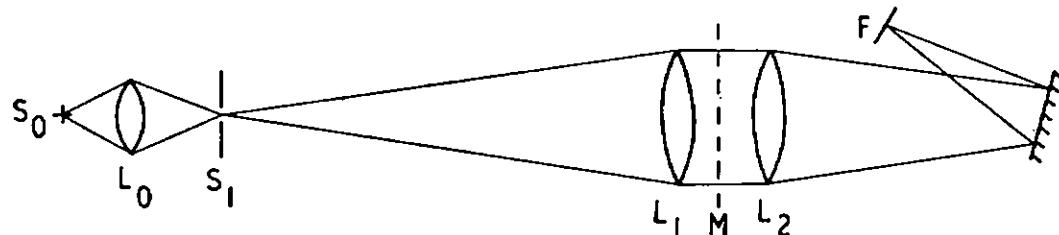


Fig. 1. The early type of diffractometer.

coherence by making the secondary source, S_1 , very small. This problem is overcome in the more recent equipment developed by Harburn and Ranniko (1972), Fig. 2, which uses a He-Ne laser as the source of light and which has been used to prepare nearly all the diffraction patterns in the Atlas.

Optically the new system differs from the old only in the nature of the source, with its near-perfect coherence and high (50mW) intensity, and the substitution of a beam expansion stage for the original condenser system. The main advantage of the higher illumination levels in the diffraction patterns is that small patterns can be considerably enlarged with a projection lens, L_3 , before being recorded photographically at F' with conveniently short exposure times. The resulting patterns are of significantly better quality than those recorded directly at F and then appreciably enlarged from the negative.

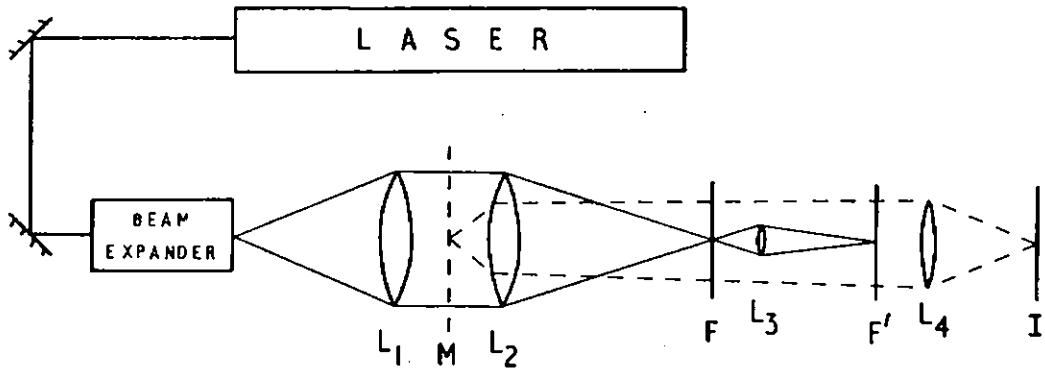


Fig. 2. The later type of diffractometer.

For some purposes it is instructive to examine an image of the mask M while it is in position between the main lenses. Such an image can be produced with an extra lens, L_4 , which, taken with L_2 , forms an image of M at I . If L_4 is beyond F , as shown in Fig. 2, the diffraction pattern can be modified by placing suitable filters in the focal plane and the consequent changes in the image observed at I . Examples of spatial filtering are shown in Plates 30–32.

The higher degree of coherence of the illumination does have some drawbacks. If there is dust on any of the optical components diffraction patterns are formed from it and these interfere with the diffraction pattern of the mask. In general, dust on the projecting lens L_3 , where the diffraction pattern of the mask covers a small area, has the most pronounced effect. The spurious fringes formed—which can be seen, for example, in Plate 29—are surprisingly difficult to eliminate. However, although unsightly, they rarely affect the interpretation of a diffraction pattern and are often tolerated in everyday work. They are evident in many of the photographs reproduced in the Atlas.

B MASKS

Masks of many different forms, prepared in a variety of ways, have been used. The simplest form of mask is made by punching out circular discs from X-ray film (Taylor and Lipson, 1964). The punch is usually mounted on a pantograph arrangement which gives a 12:1 reduction in scale from a prepared drawing to the mask. A recent development of the original pantograph has an optical projection system mounted in place of the simple punch. The projector gives a reduced image of a basic unit, which may contain up to a few hundred holes, on a photographic plate. The basic unit can be printed on the plate, in any chosen orientation in a plane, at positions specified on a prepared drawing as before. The mask is made by contact printing from the photograph on to another plate.

The original pantograph-mounted punch is satisfactory for preparing masks containing up to about 1000 holes, but is tedious to use for more than about 100 holes. A new device, the Optronics Photowrite (Harburn, Miller and Welberry, 1974), has been used to prepare all those masks which contain a very large number of holes as well as some of the smaller ones.

The Photowrite converts digital information on a magnetic tape into a distribution of optical density on a photographic film. The sheet of film, up to $10'' \times 8''$ in size, is wrapped round the outside of a cylindrical drum which can be rotated. An illuminated aperture and its 1:1 imaging system is mounted on a carriage which can move parallel to the rotation axis of the drum so that the whole film is scanned in a raster fashion by the light beam. The film can only be exposed at the nodes of a square lattice but up to 8×10^7 dots can be printed on a full sheet of film. Like the masks produced with the modified pantograph arrangement, those made with the Photowrite are in the form of photographic plates or films. It is not normally possible to use such masks directly in the diffractometer because variations in the optical thickness of the emulsion and its support give phase errors which spoil the diffraction patterns. In such circumstances the mask has to be used in an optical gate (Harburn and Ranniko, 1971) which consists of an oil, chosen so that its refractive index closely matches those of the emulsion and support, contained between two pieces of glass the outer surfaces of which are flat to about $\lambda/20$.

Alternatively, and provided that the photographic mask does not contain any isolated 'opaque' regions, an etching in copper foil can be made from it. The procedure has been described in detail by Hill and Rigby (1969), its essential features are as follows. A piece of copper foil, secured to a sheet of inert material, is thoroughly cleaned and coated with a thin film of photoresist which is warmed until it is hard and dry. A contact print is made from a photographic negative of the mask using ultra-violet light which makes the resist insoluble in a special developer. The resist which has not been hardened is removed by the developer and the exposed copper is electroplated with a thin film of nickel. The remainder of the resist is then removed with paint stripper and the copper beneath it is dissolved with an etchant which does not attack the nickel. Finally, the foil is removed from the backing sheet. The nickel film ensures that the outlines of the required apertures are preserved unaffected by undercutting of the copper during etching. Etched masks are preferred to photographic plates used in the optical gate. The latter procedure is messy, whereas the etched masks are always immediately available and have unobstructed apertures which cannot affect the phase of the light beams transmitted through them.

Several of the plates show masks in which the amplitudes or phases (or both) of the beams transmitted through the apertures have been changed deliberately. The methods for effecting such changes have been fully described by Harburn (1973). For ease of reference in the notes on the plates the various methods are listed below.

Amplitude control

1. Holes of different sizes.
2. Gauzes of different transmissions.
3. Mica half-wave plates oriented in plane-polarised light.

Phase control

4. Mica plates oriented in unpolarised light. Phases 0 and π only.
5. Mica half-wave plates oriented in plane-polarised light phases 0 and π only.

6. Mica plates tilted in unpolarised light. Phases 0 to 2π in principle, but only 0 to π in practice.
7. Mica half-wave plates oriented in circularly-polarised light. All phases in the full 0 to 2π range.

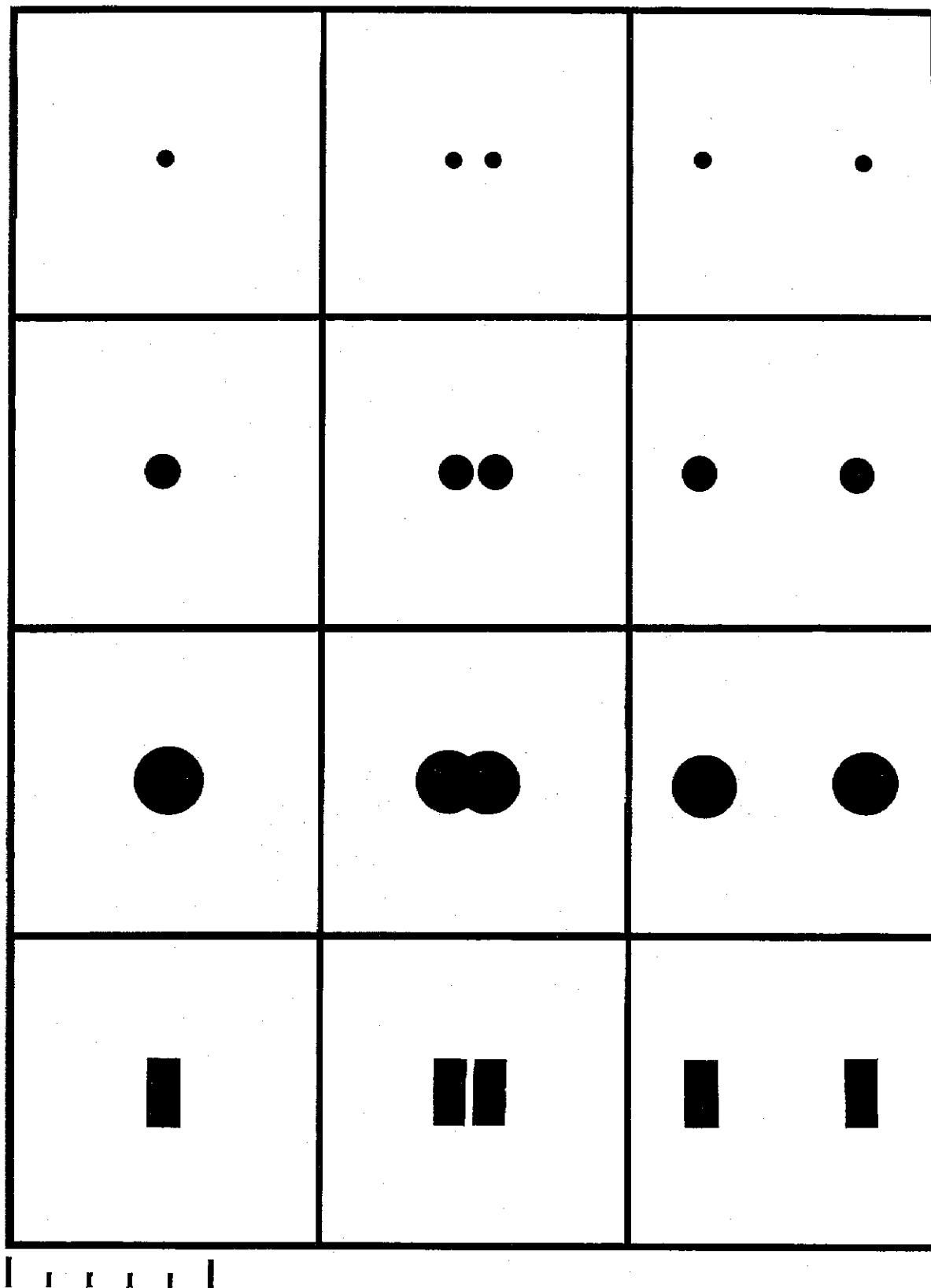
The pieces of gauze and mica are usually mounted on small brass plugs which fit into holes in the mask plate.

C PHOTOGRAPHY

Exposure times for photographs taken on the latest diffractometer are generally short. About 1/60 s is typical but exposures as long as 4 minutes and as short as 1/750 s, with the main beam intensity reduced with a polaroid filter, have been used. A Pentax 35mm camera body is used to expose the film which must be red sensitive. Ilford Pan F and FP4 are used most often, developed in either Kodak D19 or Ilford ID11 depending on the contrast required in the negative.

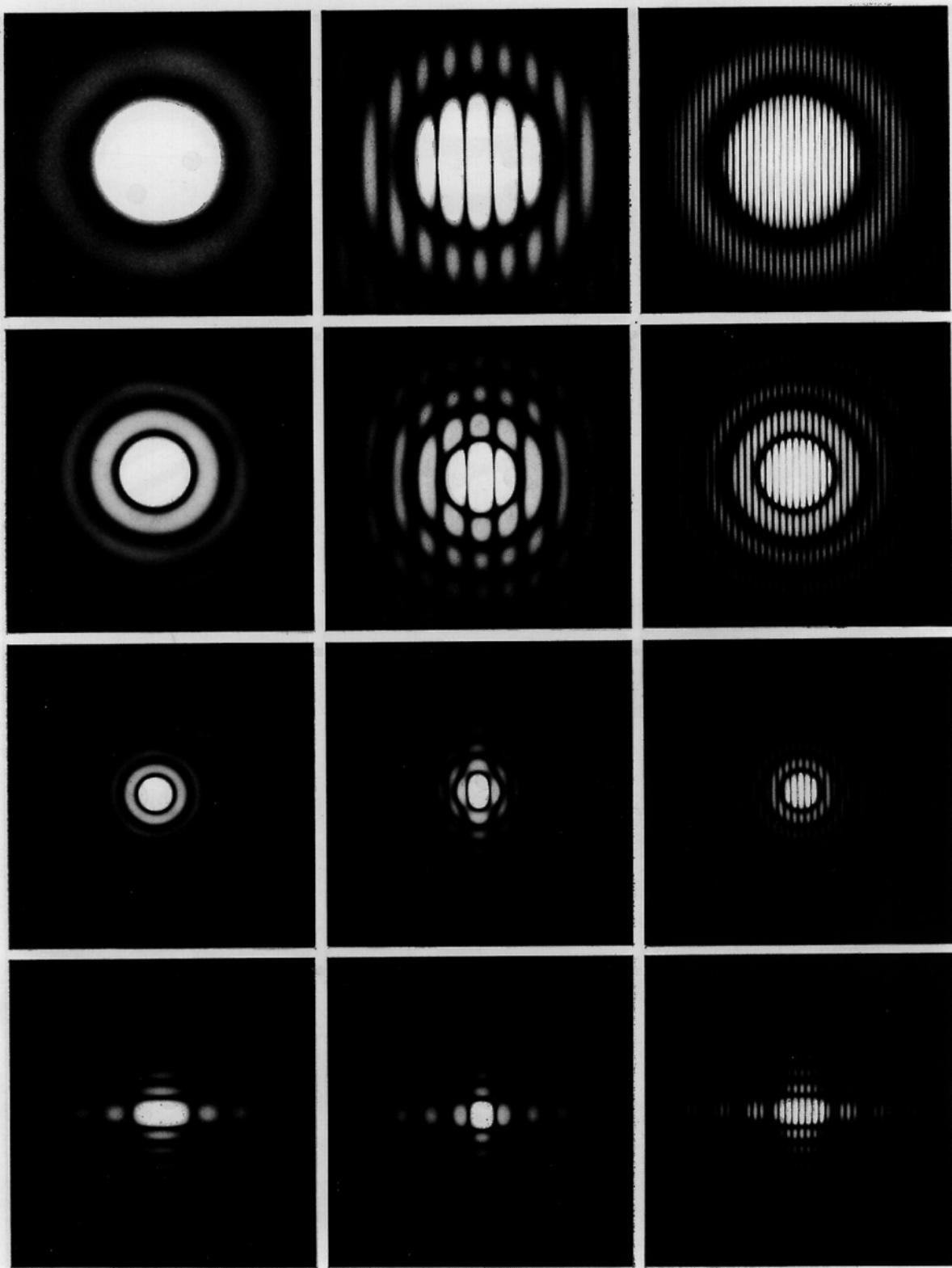
All the photographs are enlargements, usually less than 5 \times , from 35mm negatives. In the few cases where photographs have been taken on the older type of diffractometer the enlargements from the negatives may be as much as 50 \times .

Plate 1



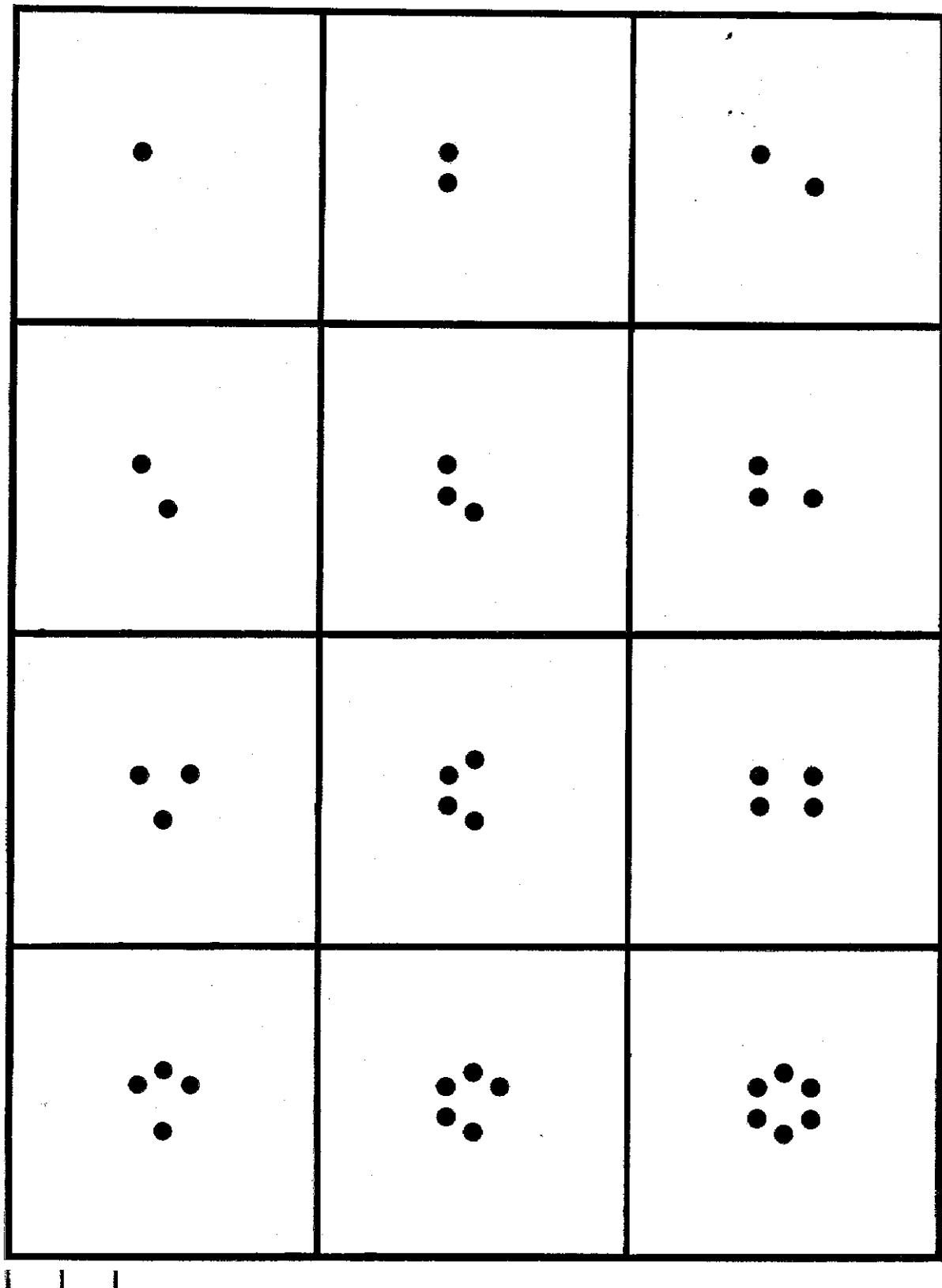
1 2 3 4 5 6

Plate I



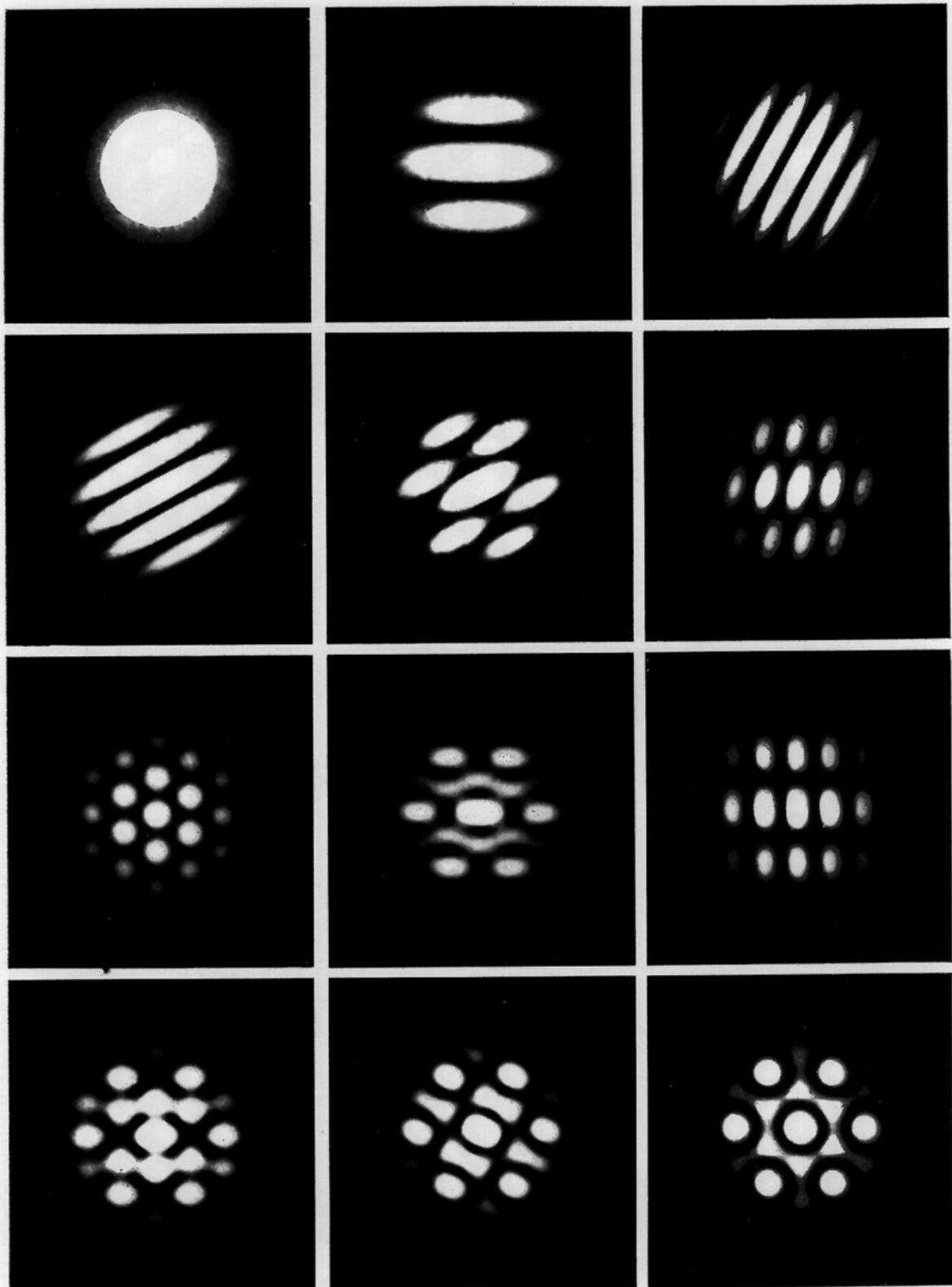
I II III

Plate 2



|||

Plate 2



1 2 3 4 5 6

Plate 3

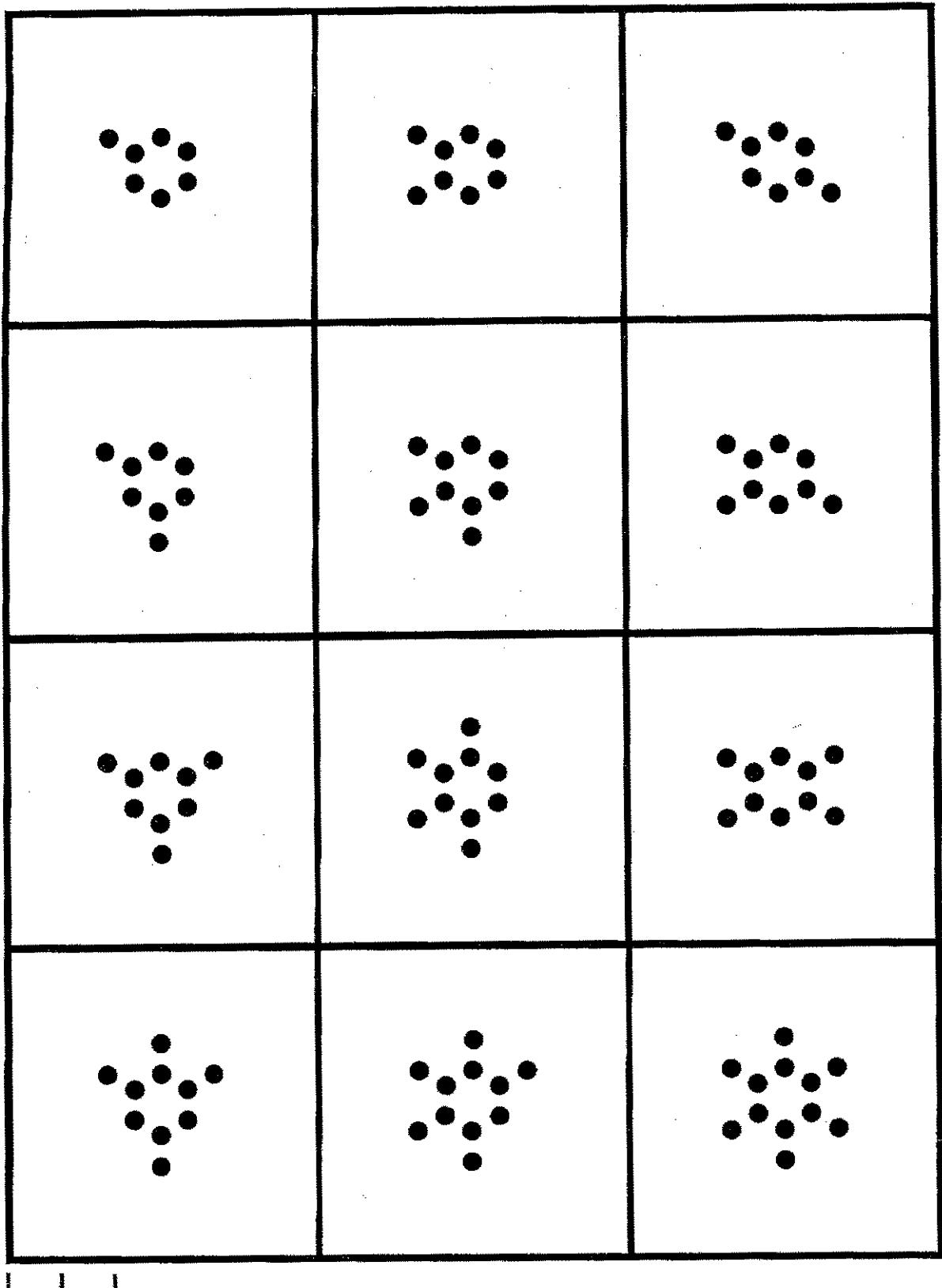
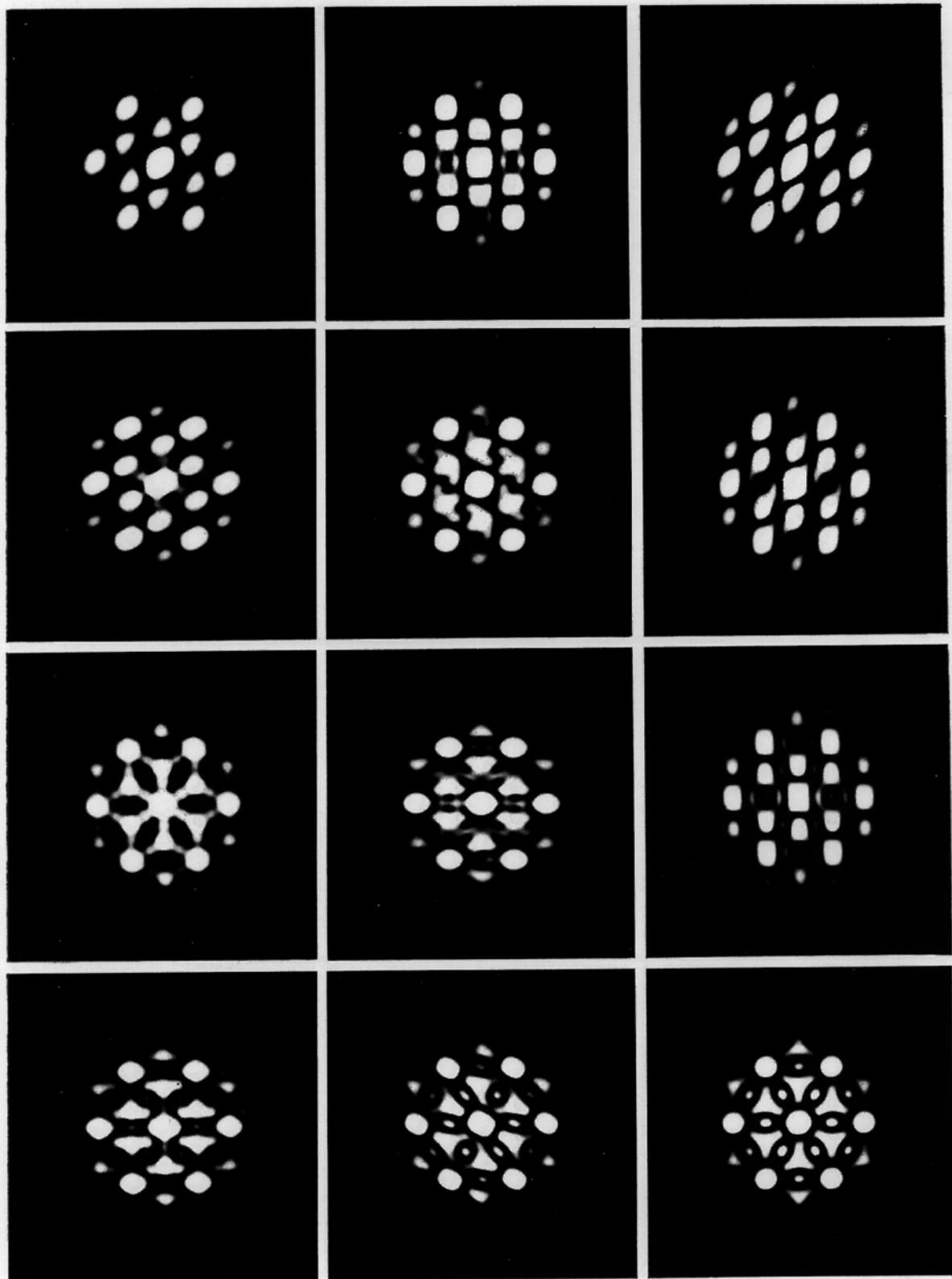
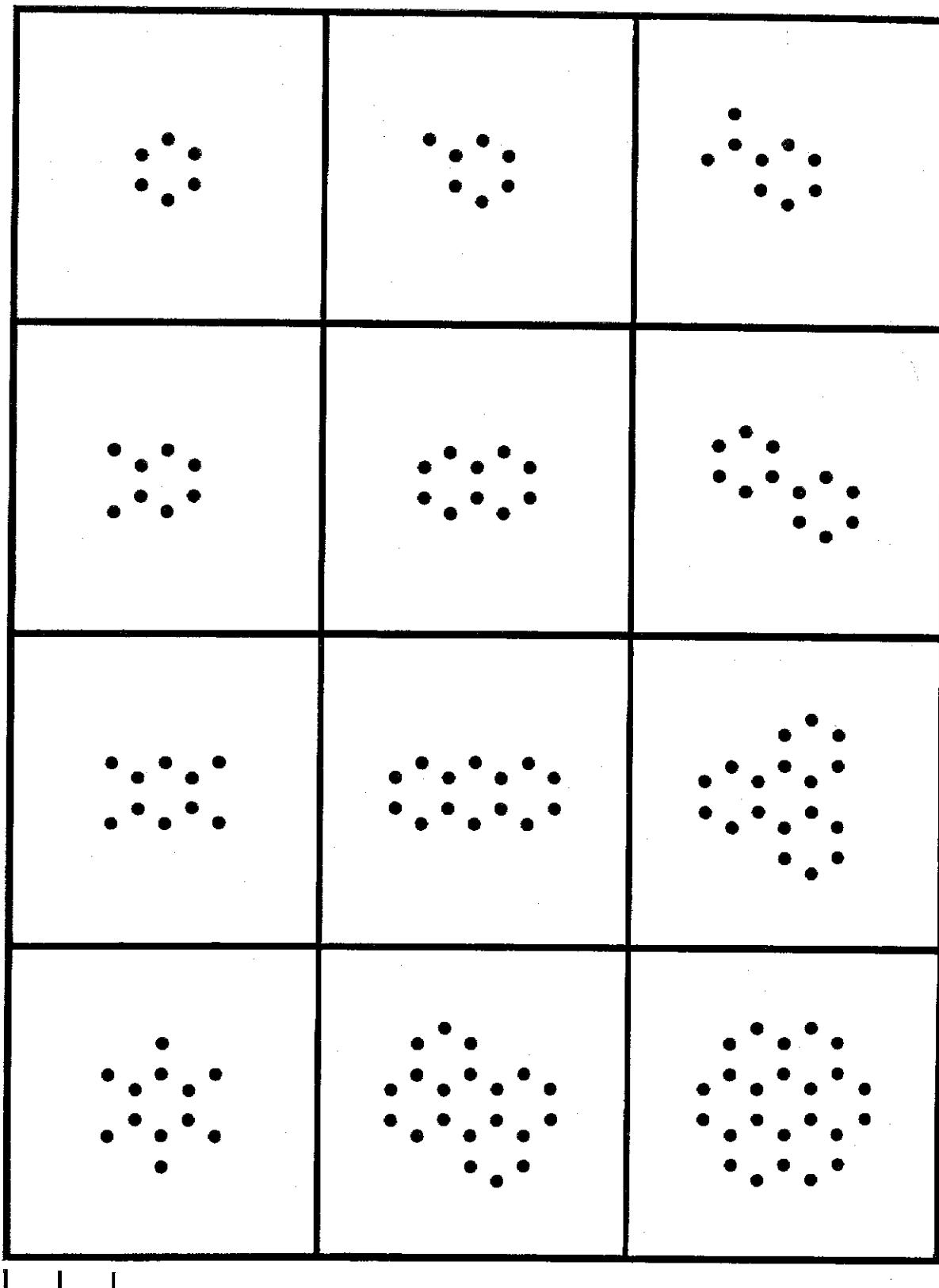


Plate 3



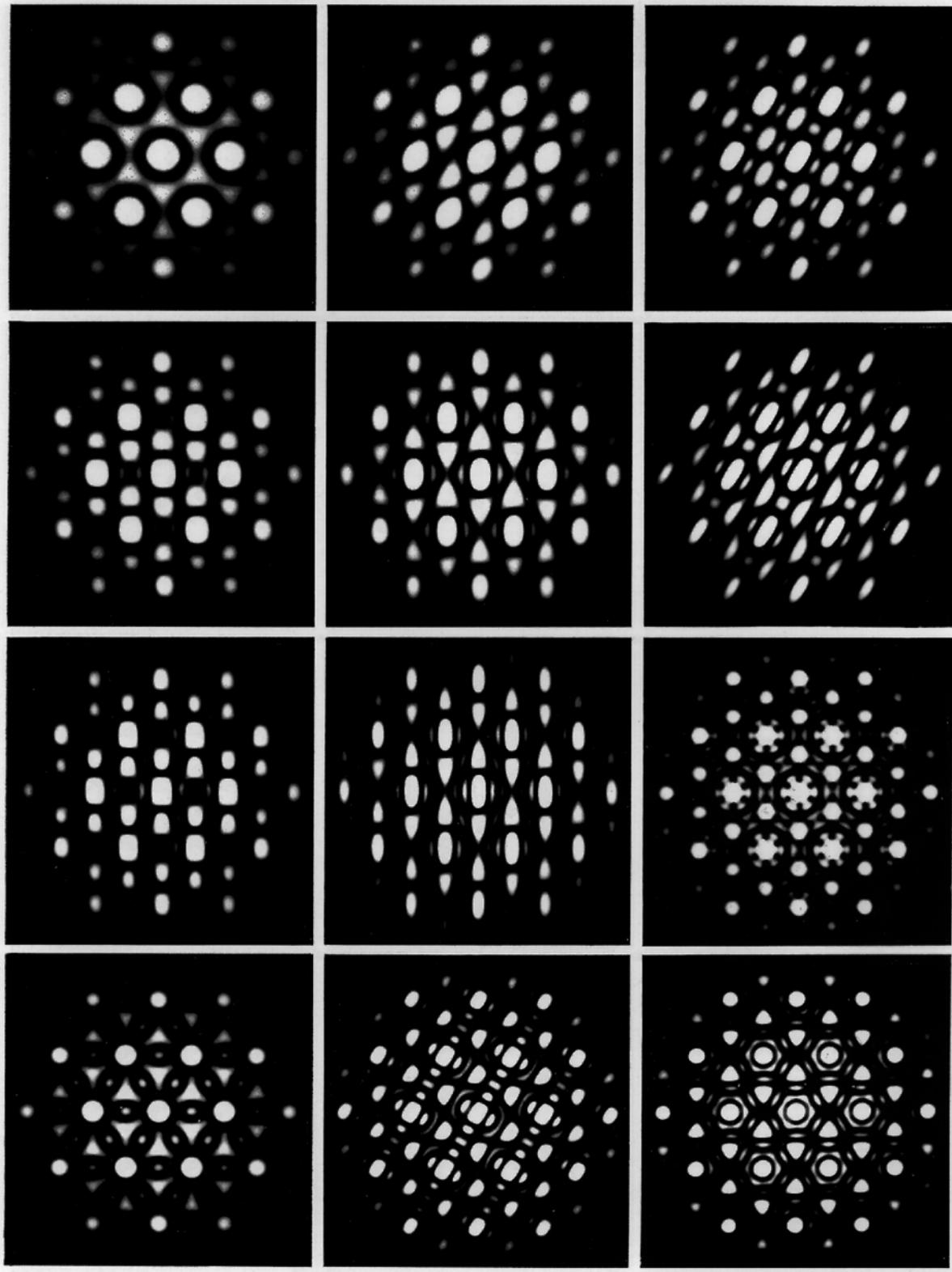
1 2 3 4 5 6

Plate 4



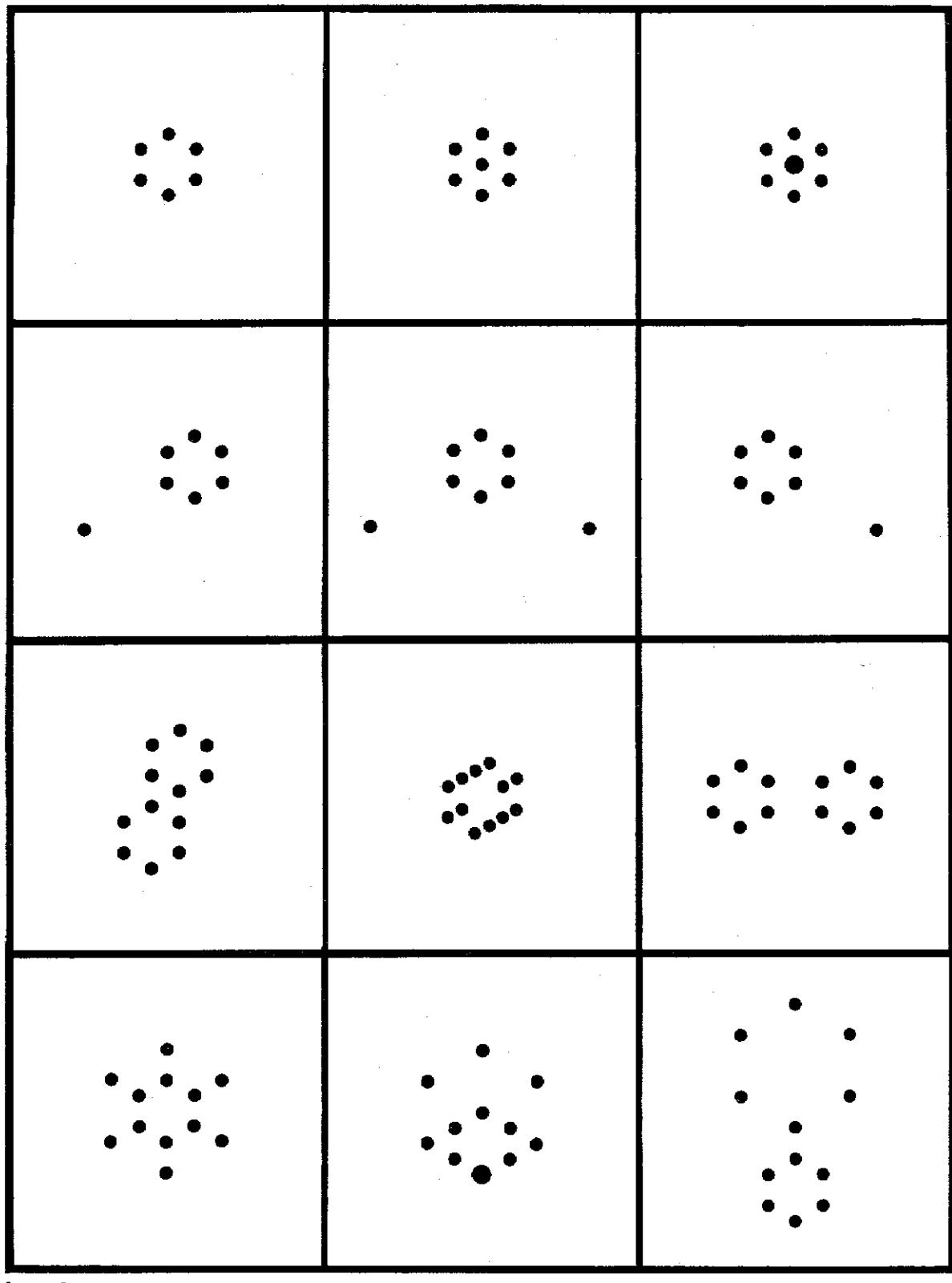
1 1 1

Plate 4



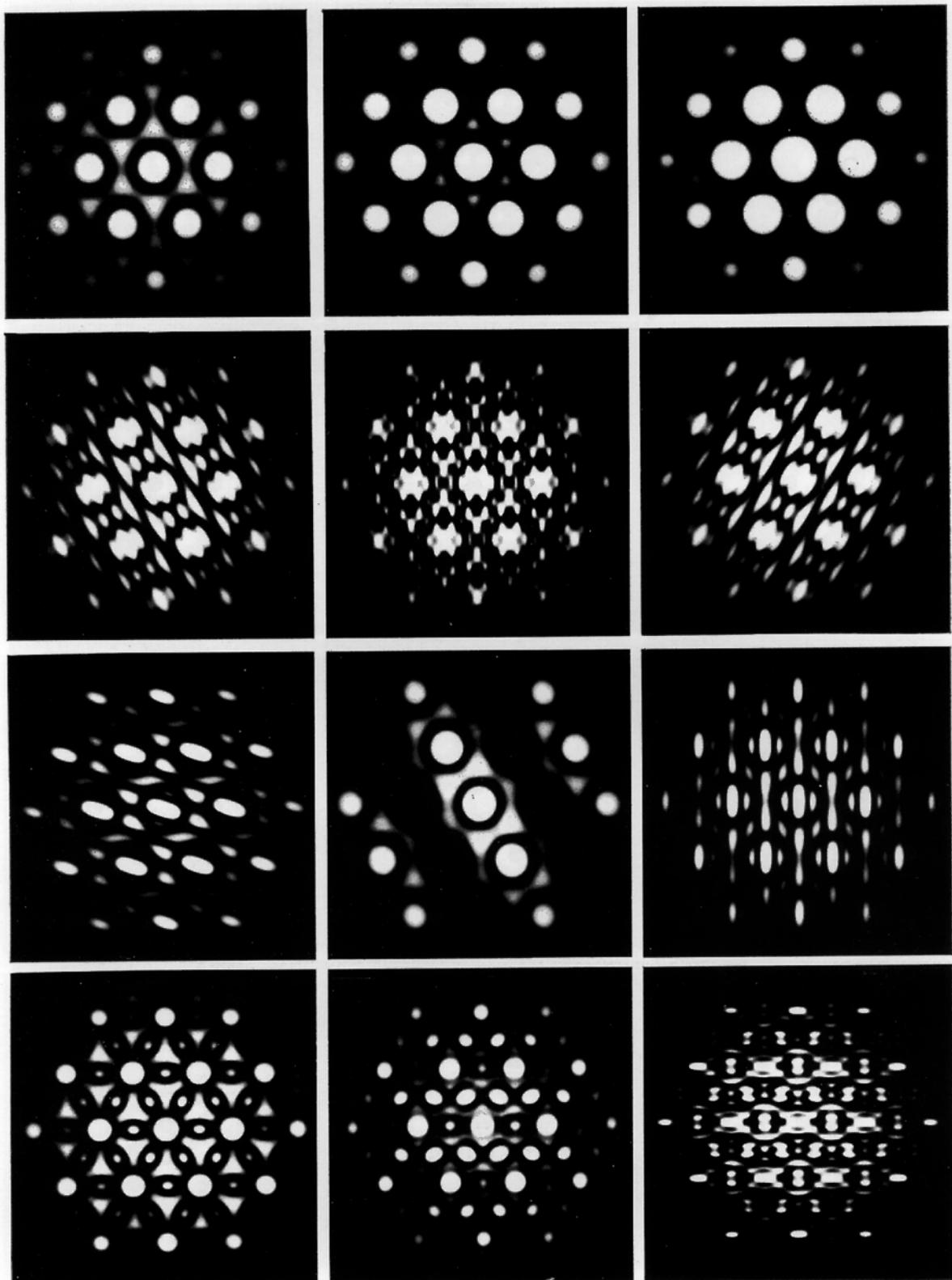
1 2 3 4 5 6

Plate 5



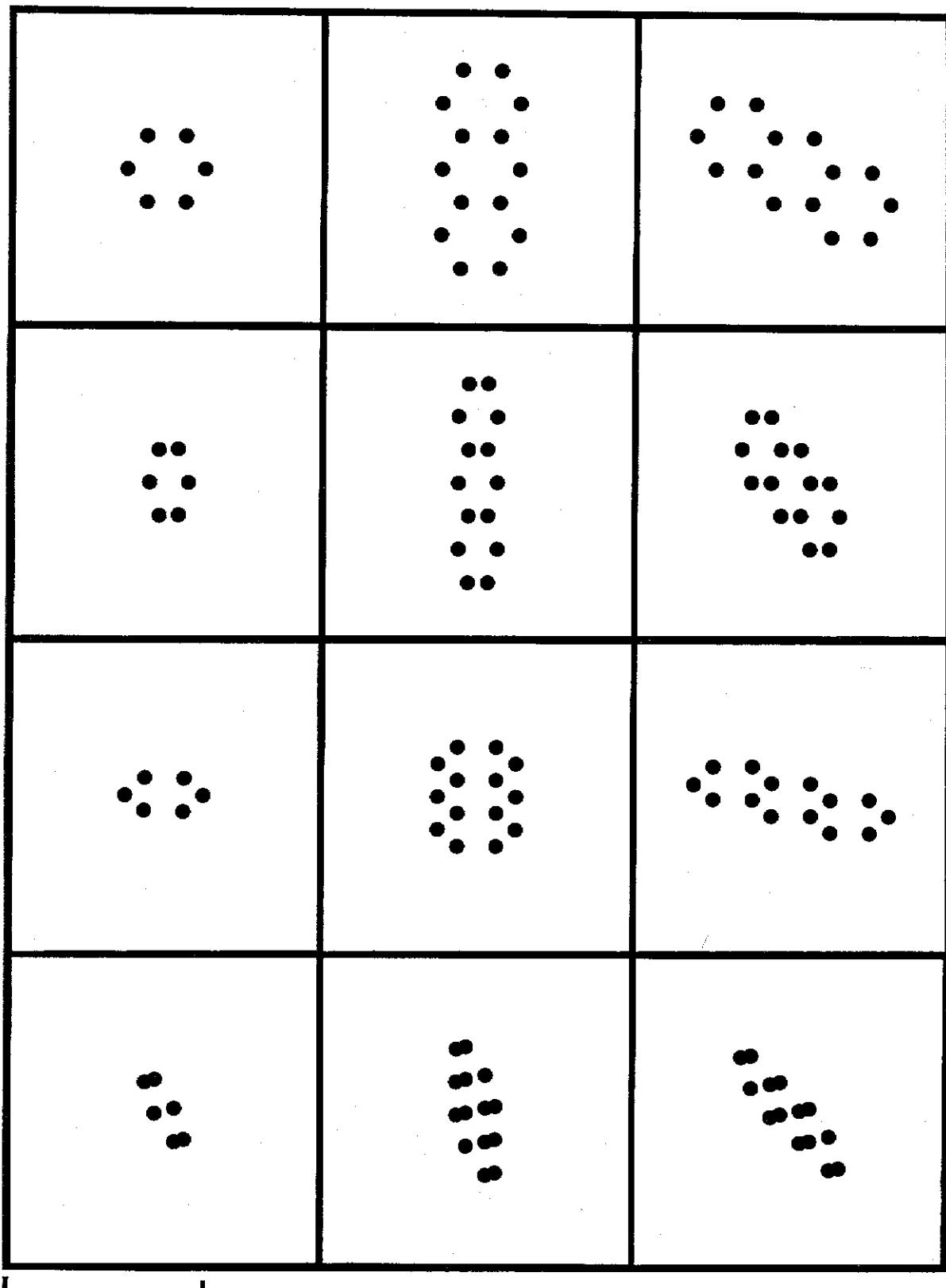
| | |

Plate 5



1 2 3 4 5 6

Plate 6



1 2 3 4 5 6

Plate 6

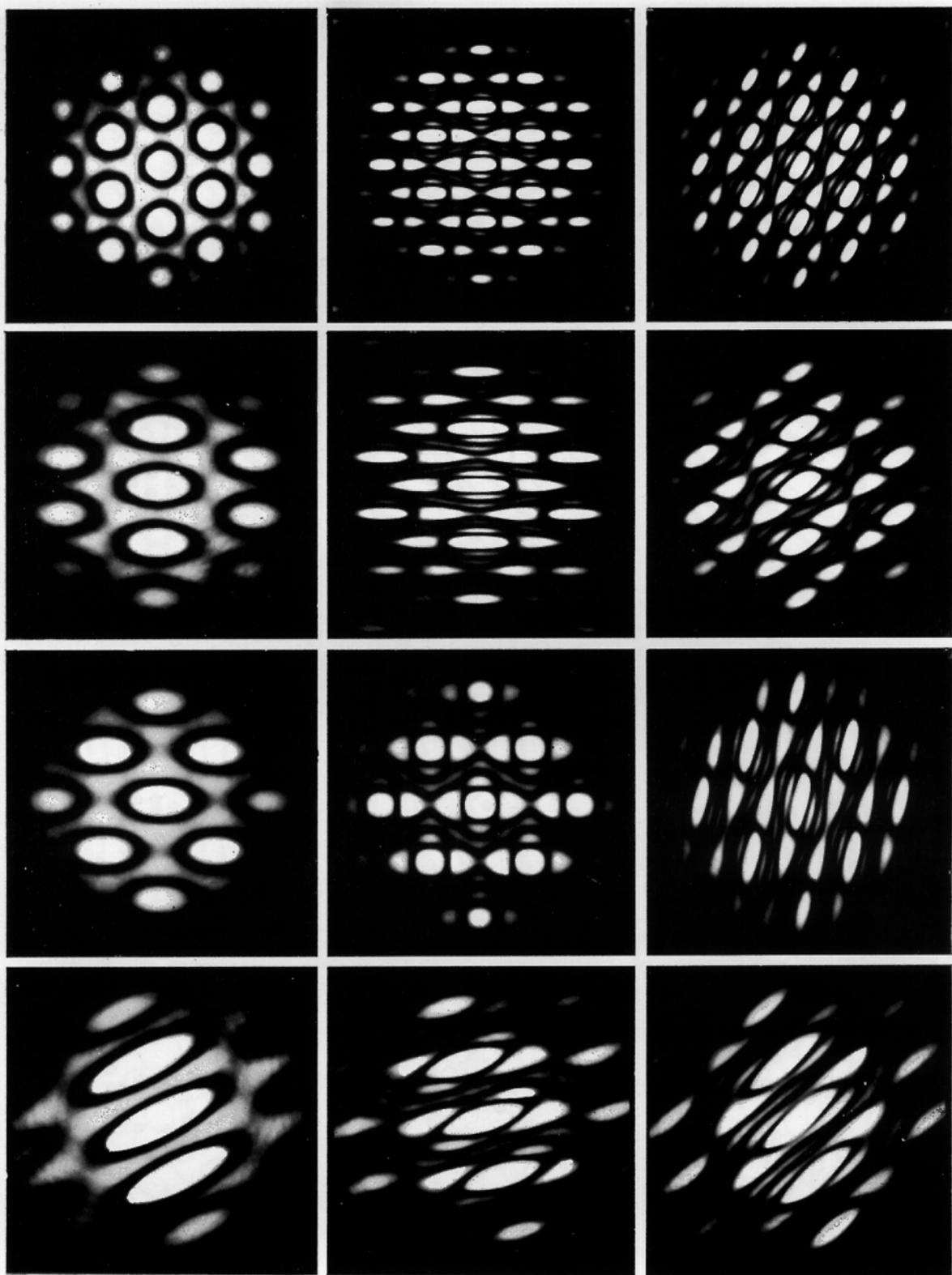
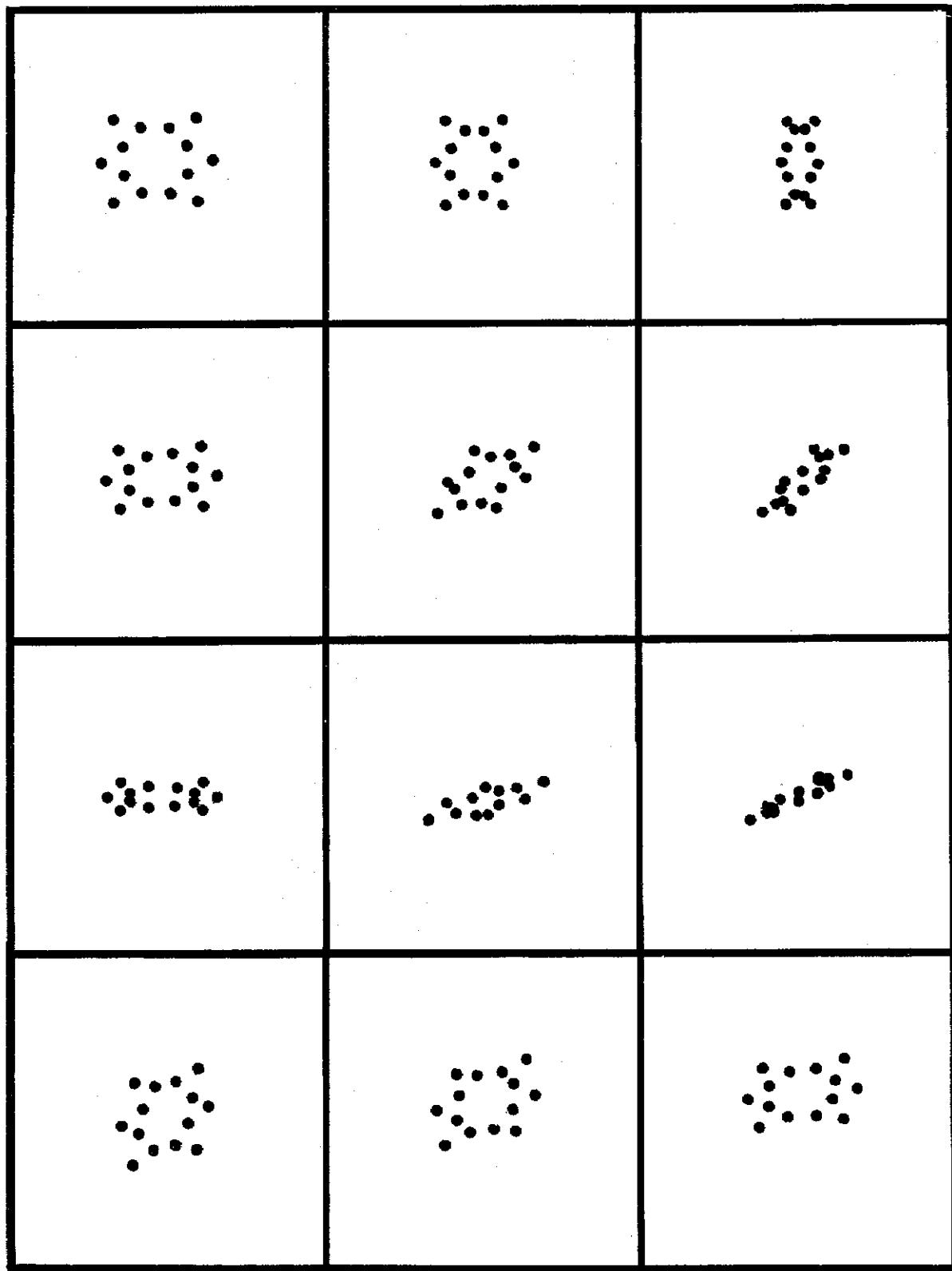


Plate 7



1 mm

Plate 7

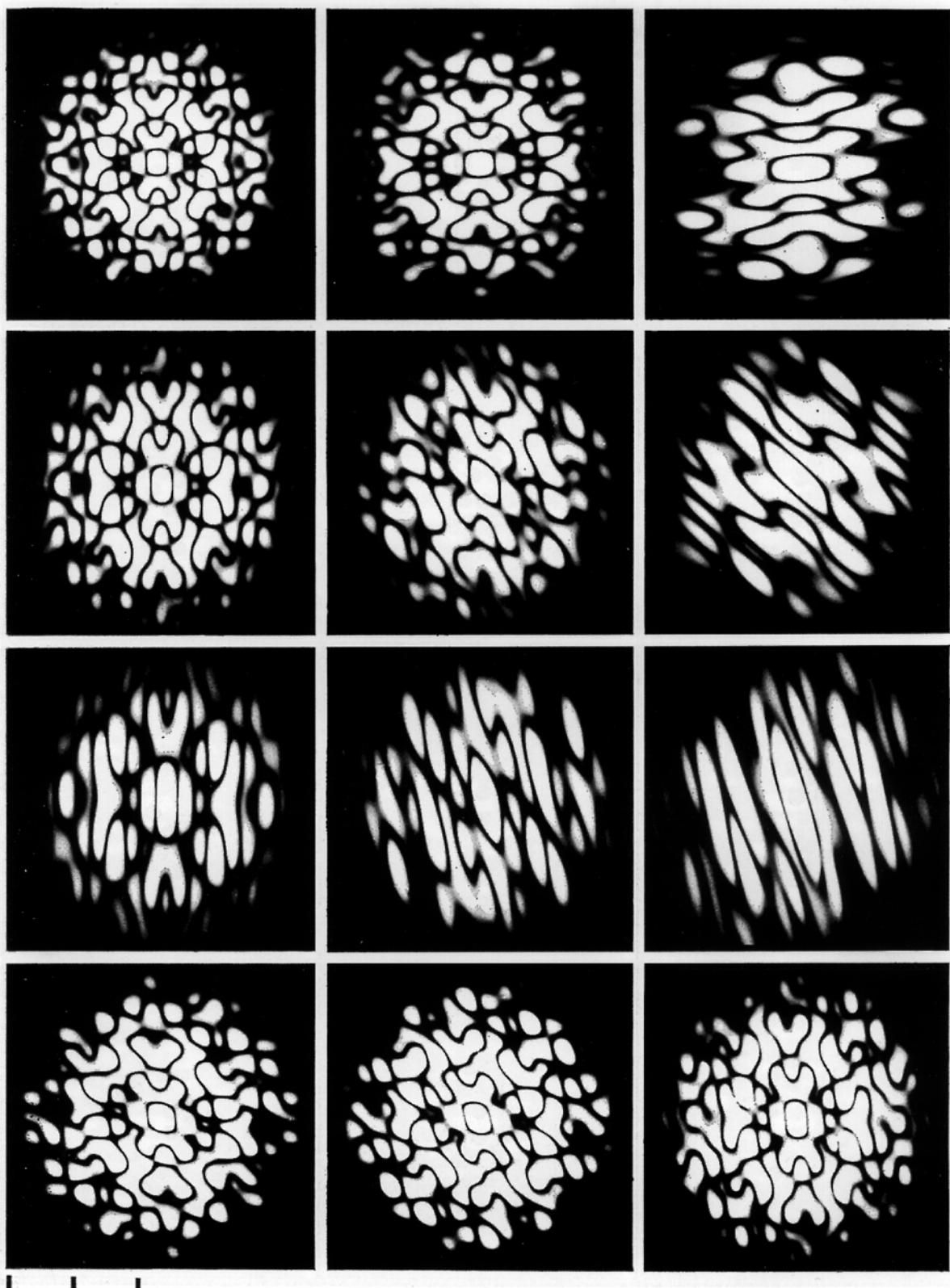


Plate 8

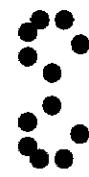
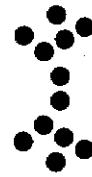
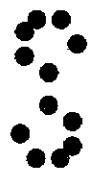
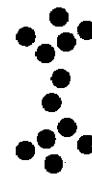
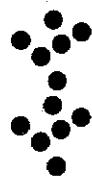
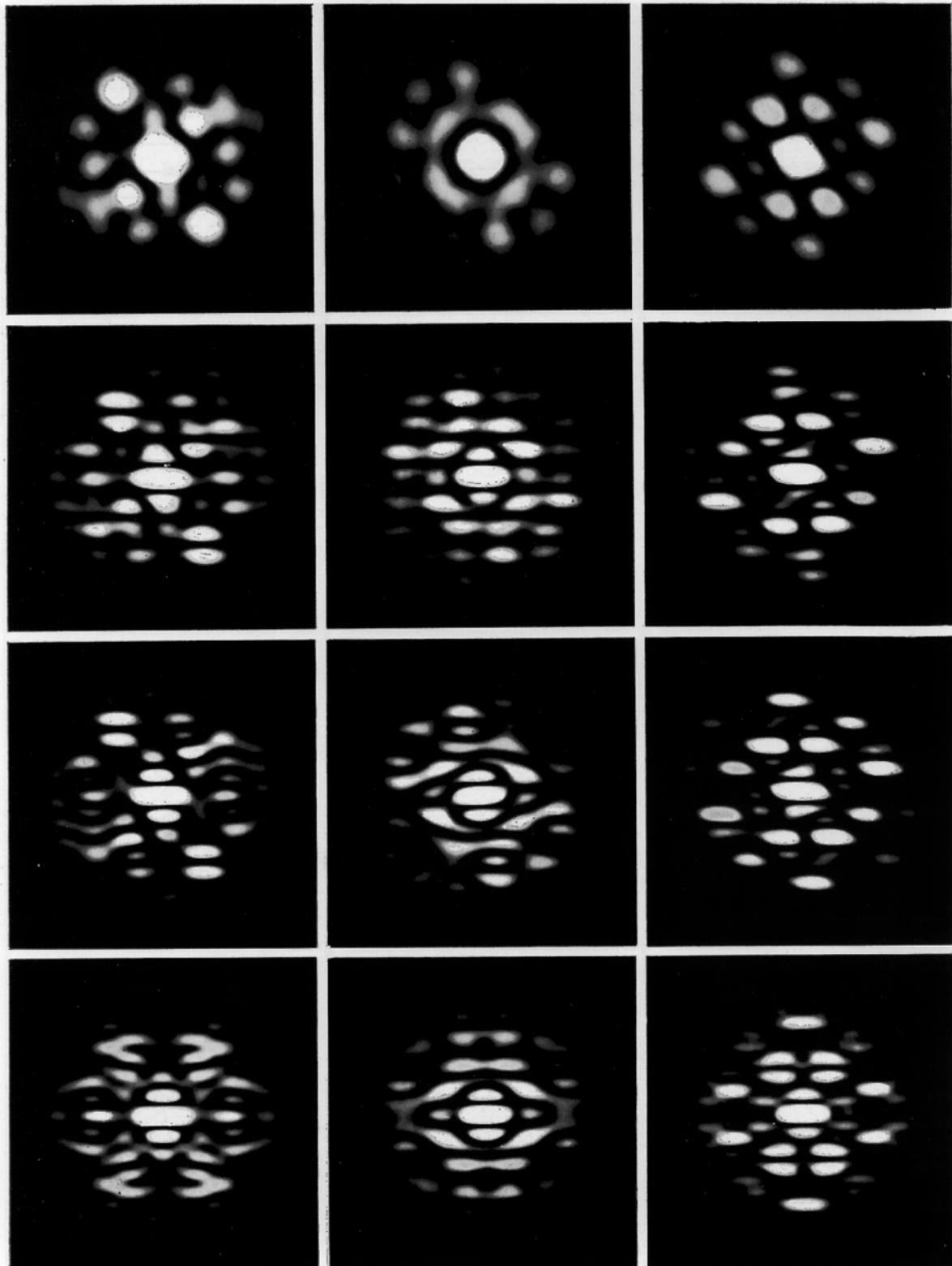


Plate 8



1 mm

Plate 9

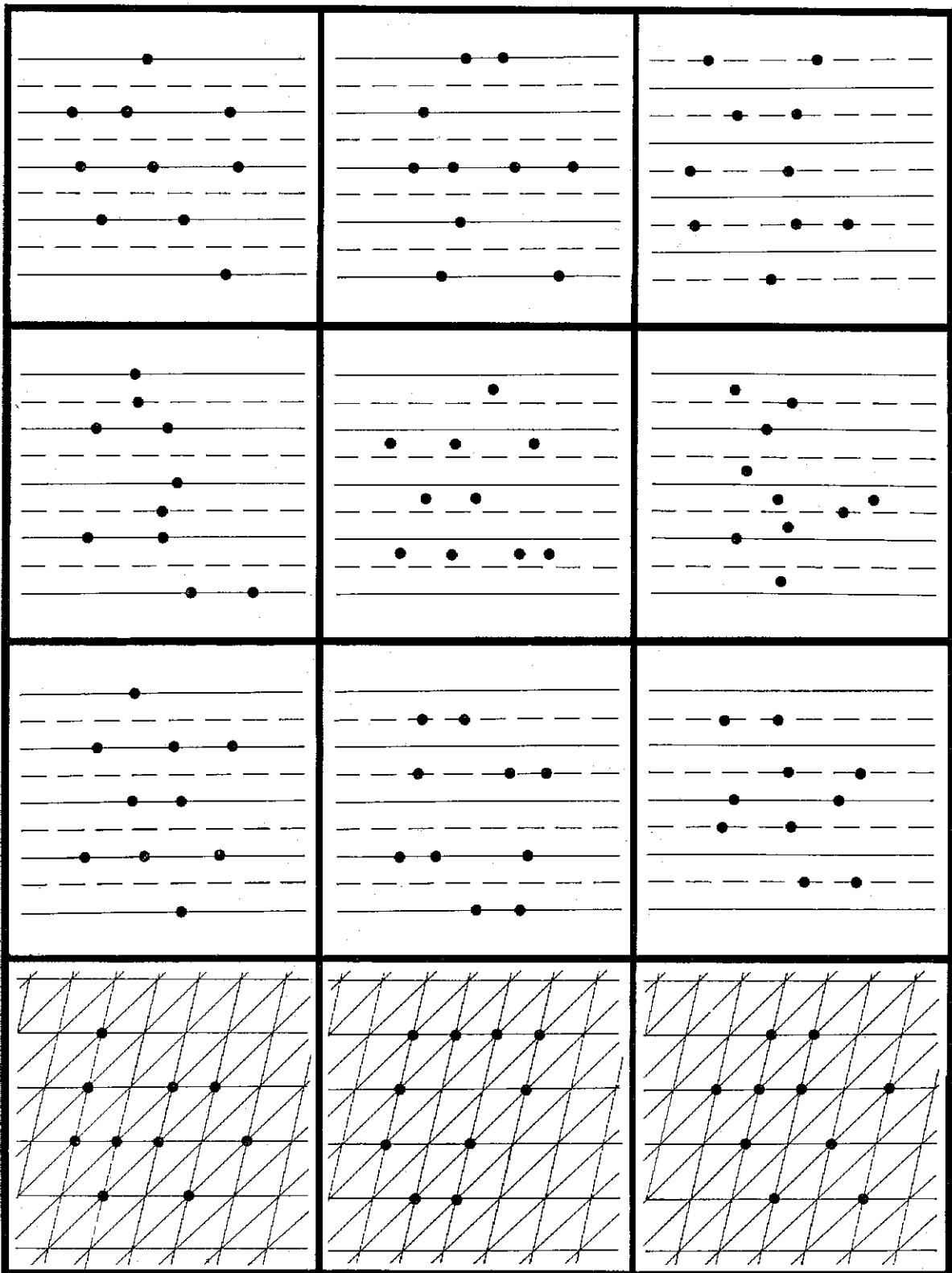
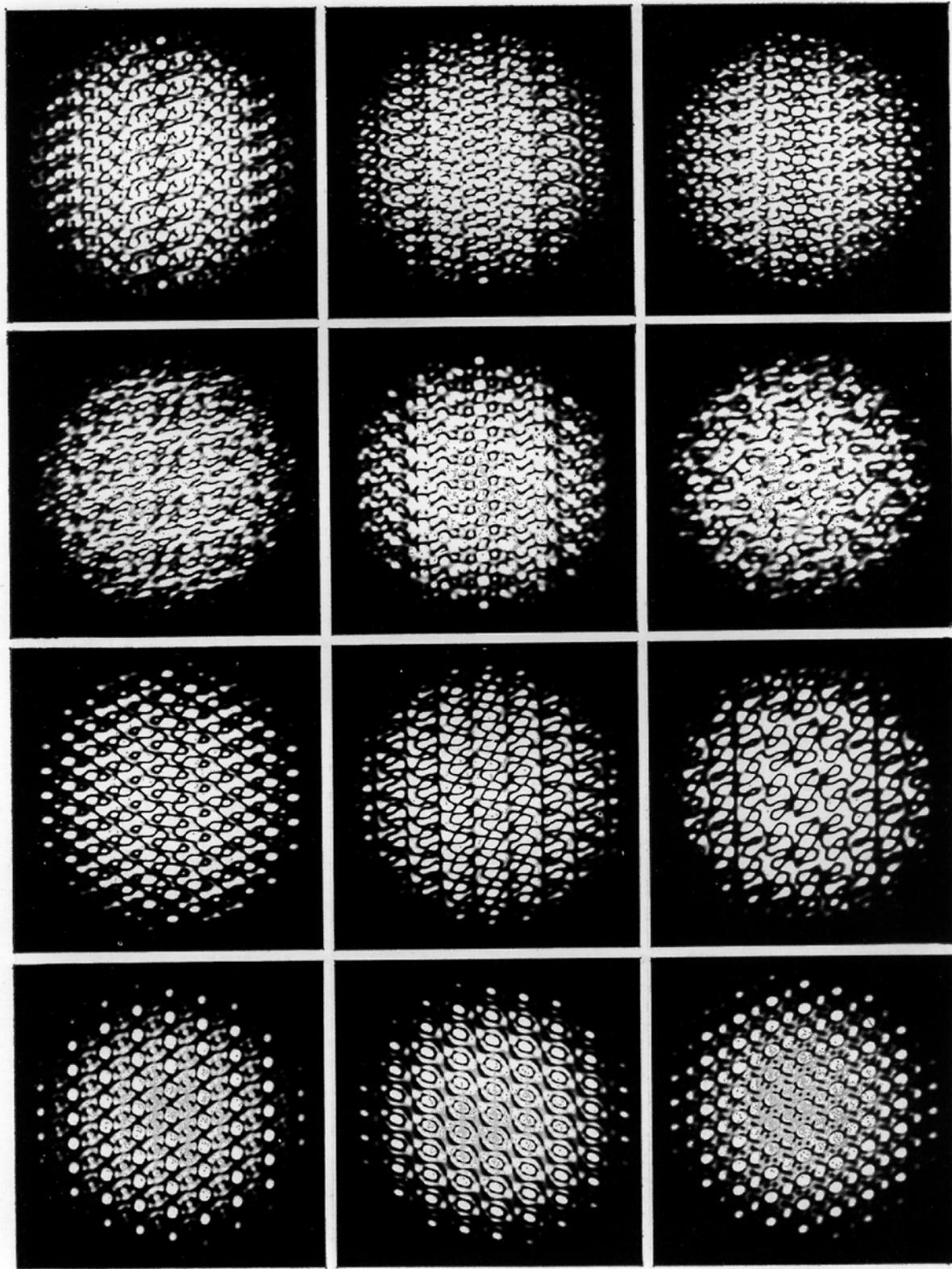


Plate 9



1 2 3 4 5 6

Plate 10

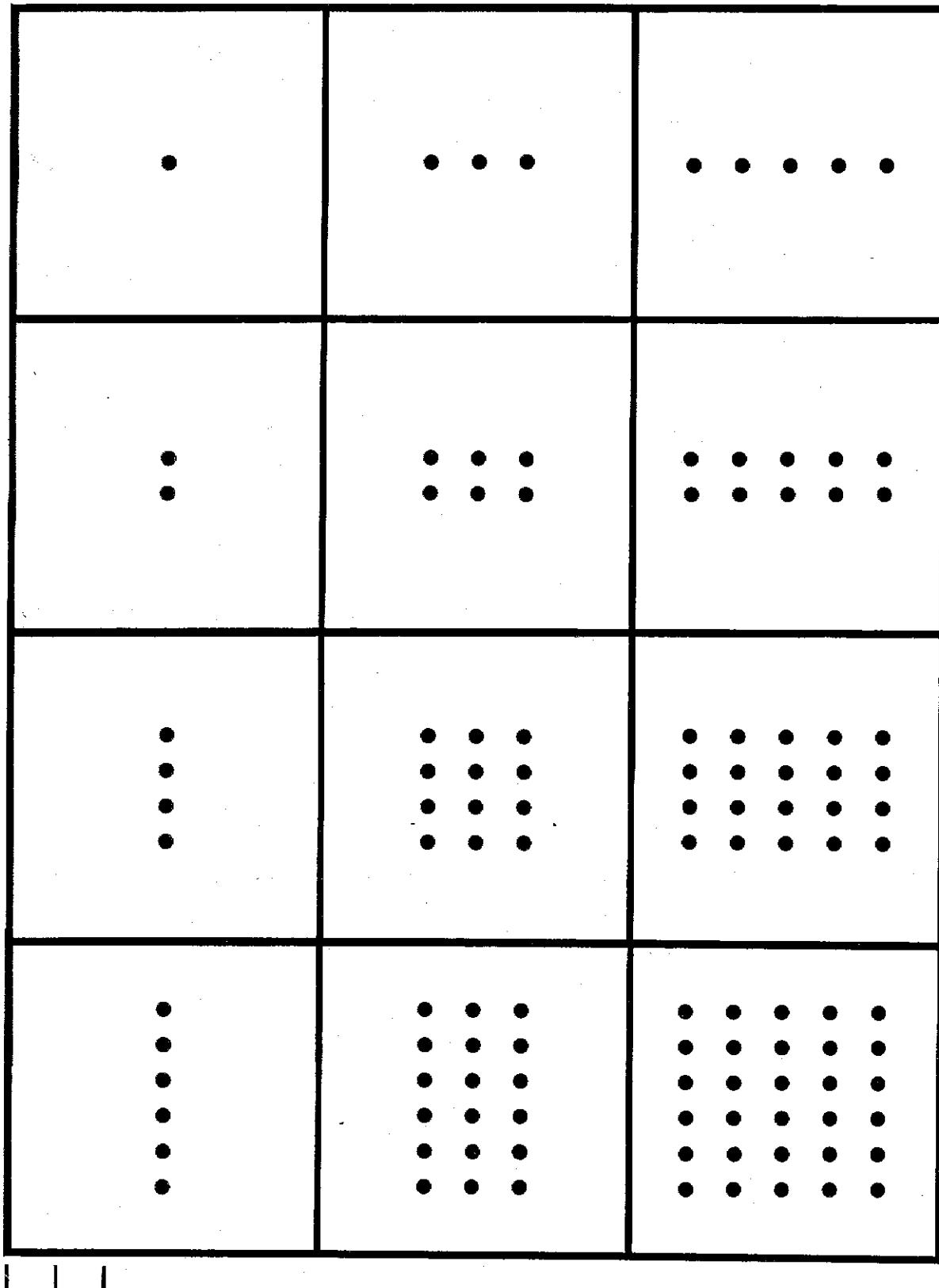
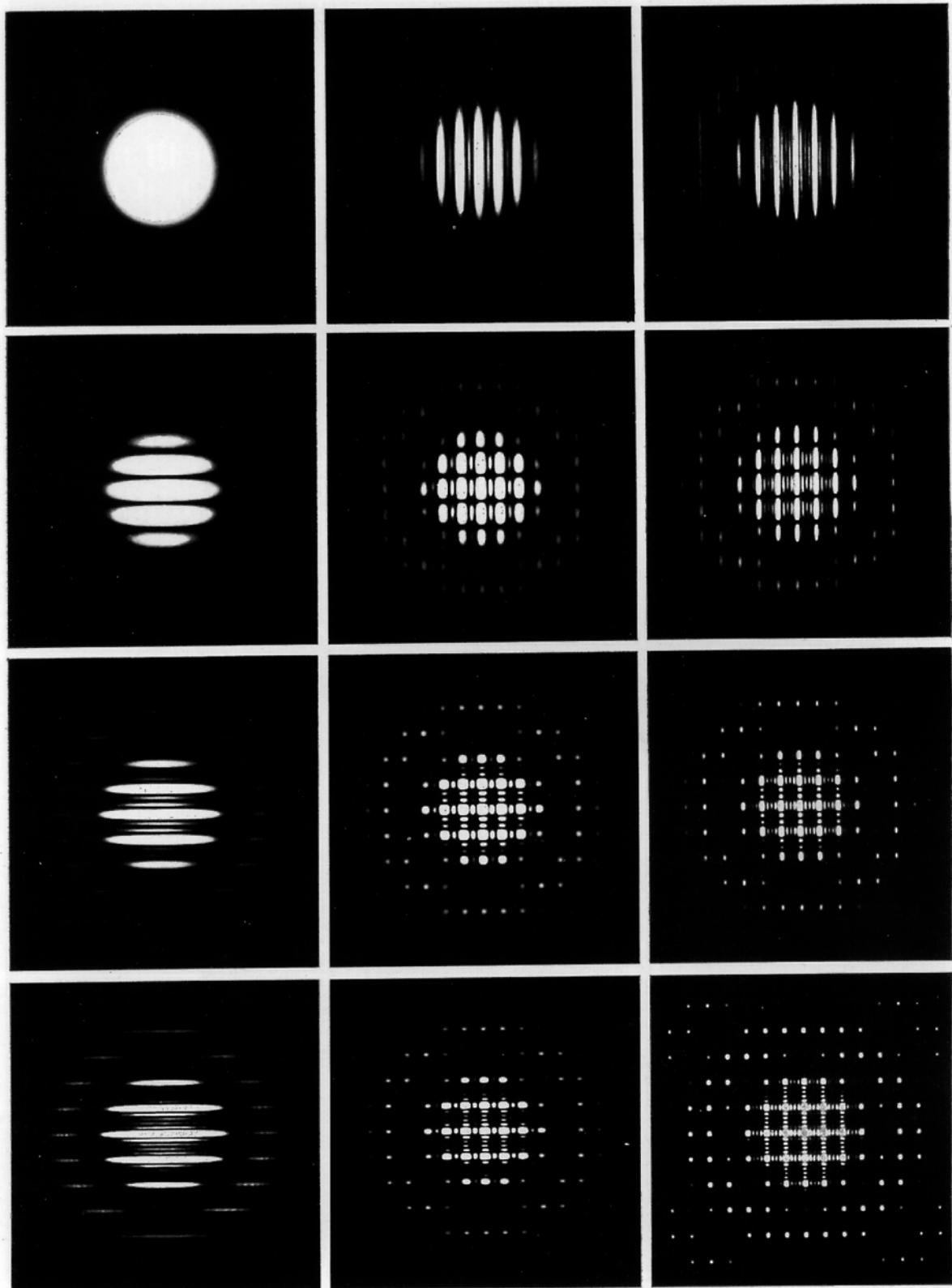
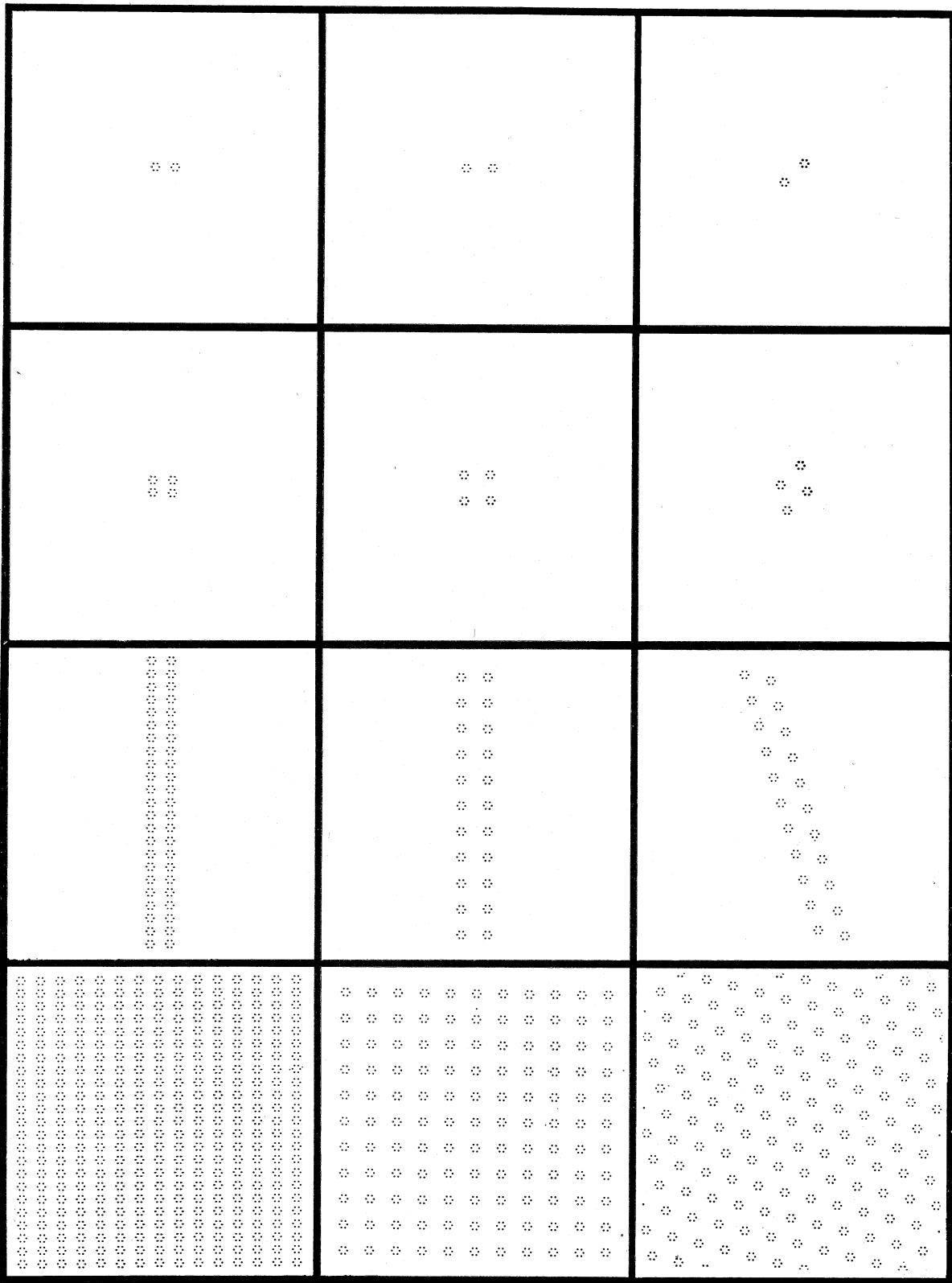


Plate 10



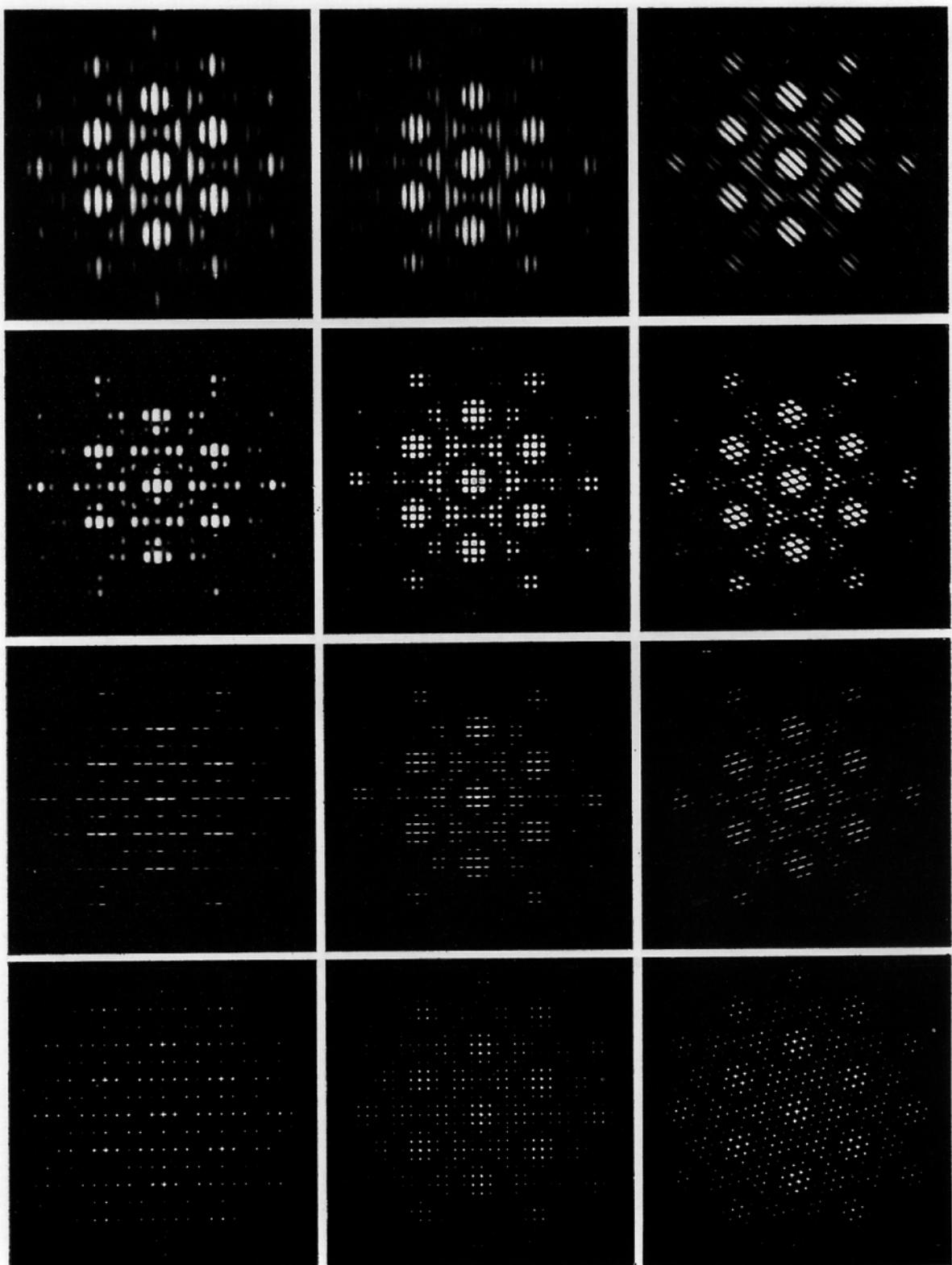
111111

Plate II



[.....]

Plate 11



lou lou

Plate 12

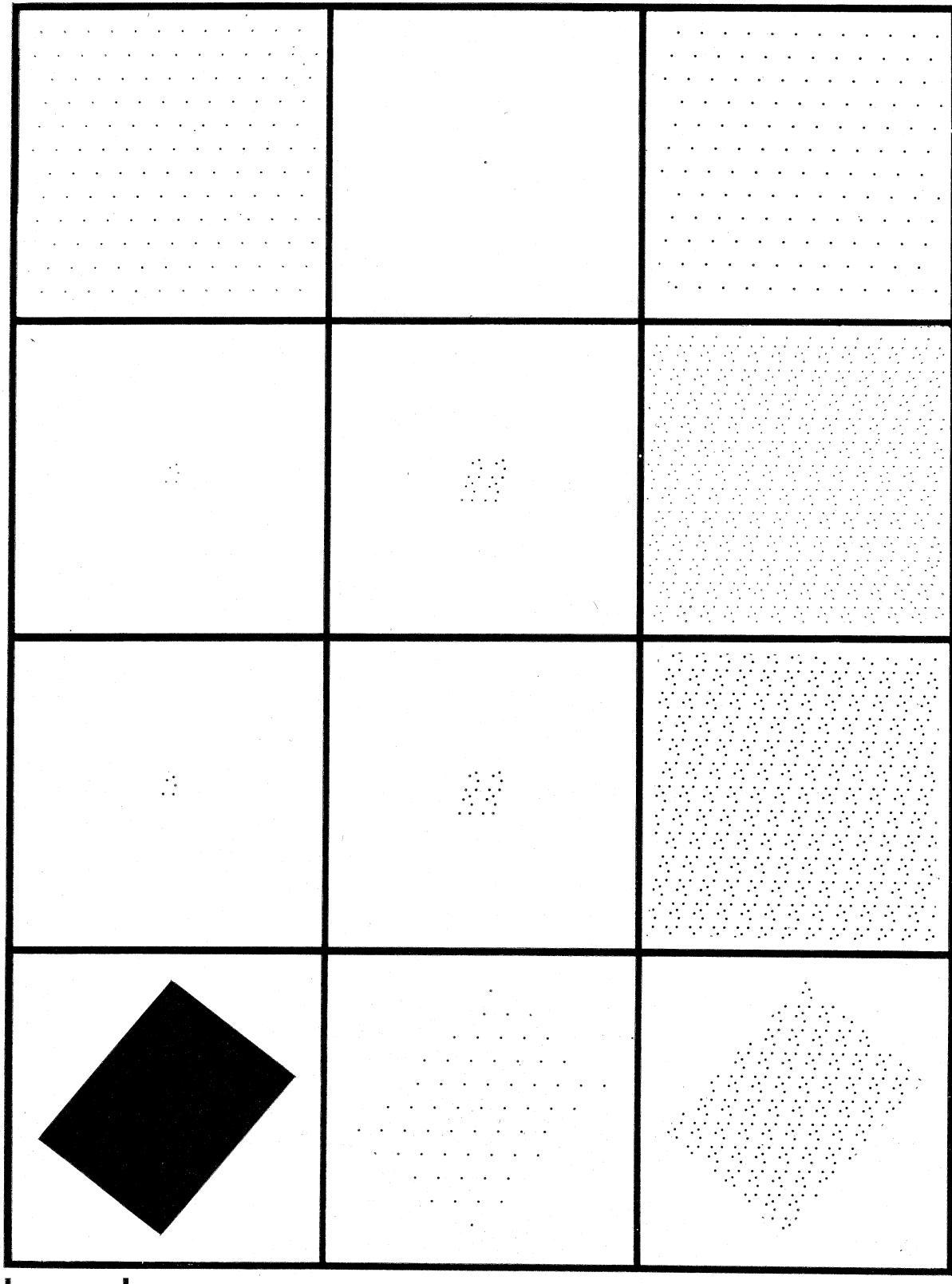
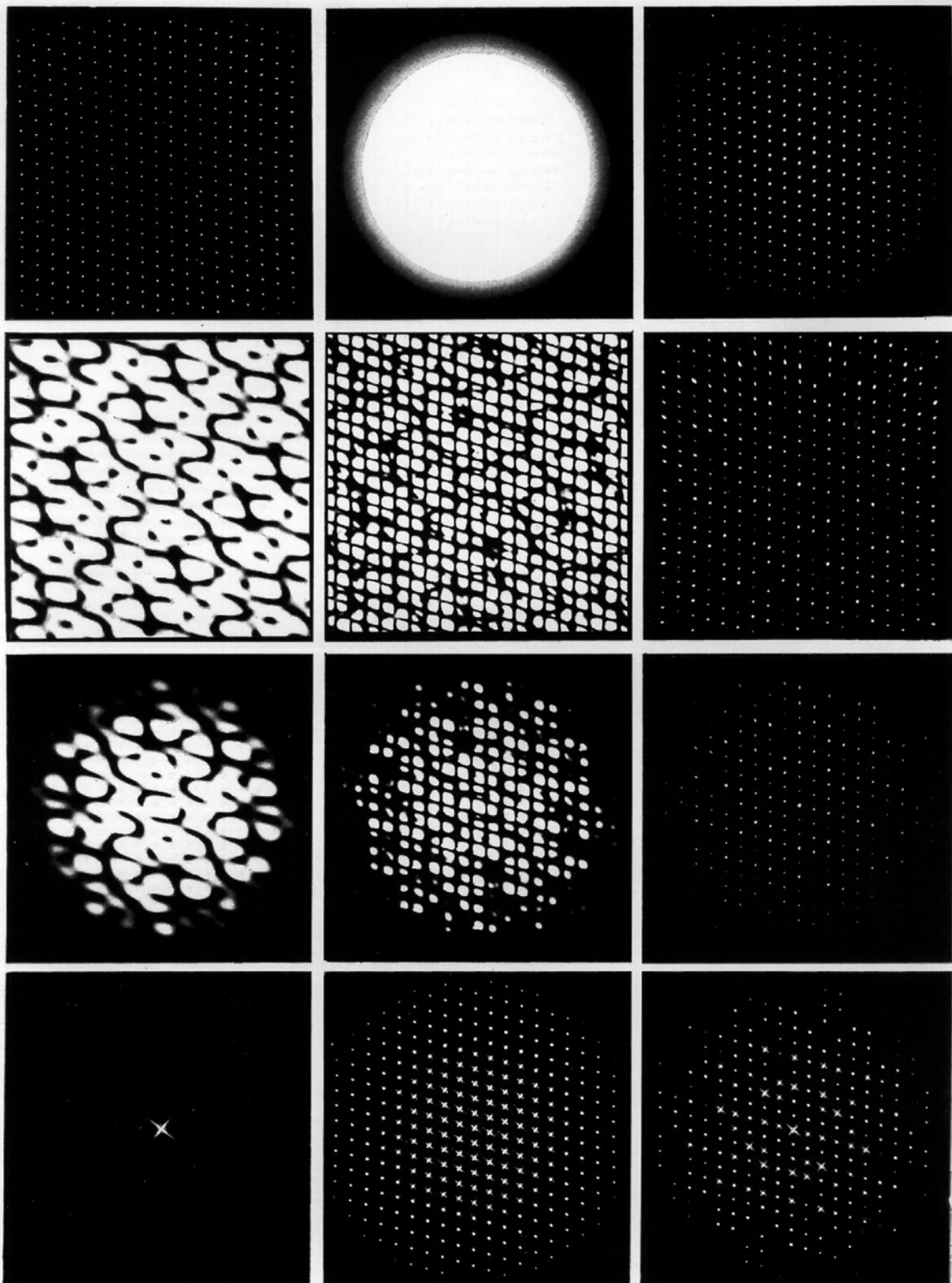
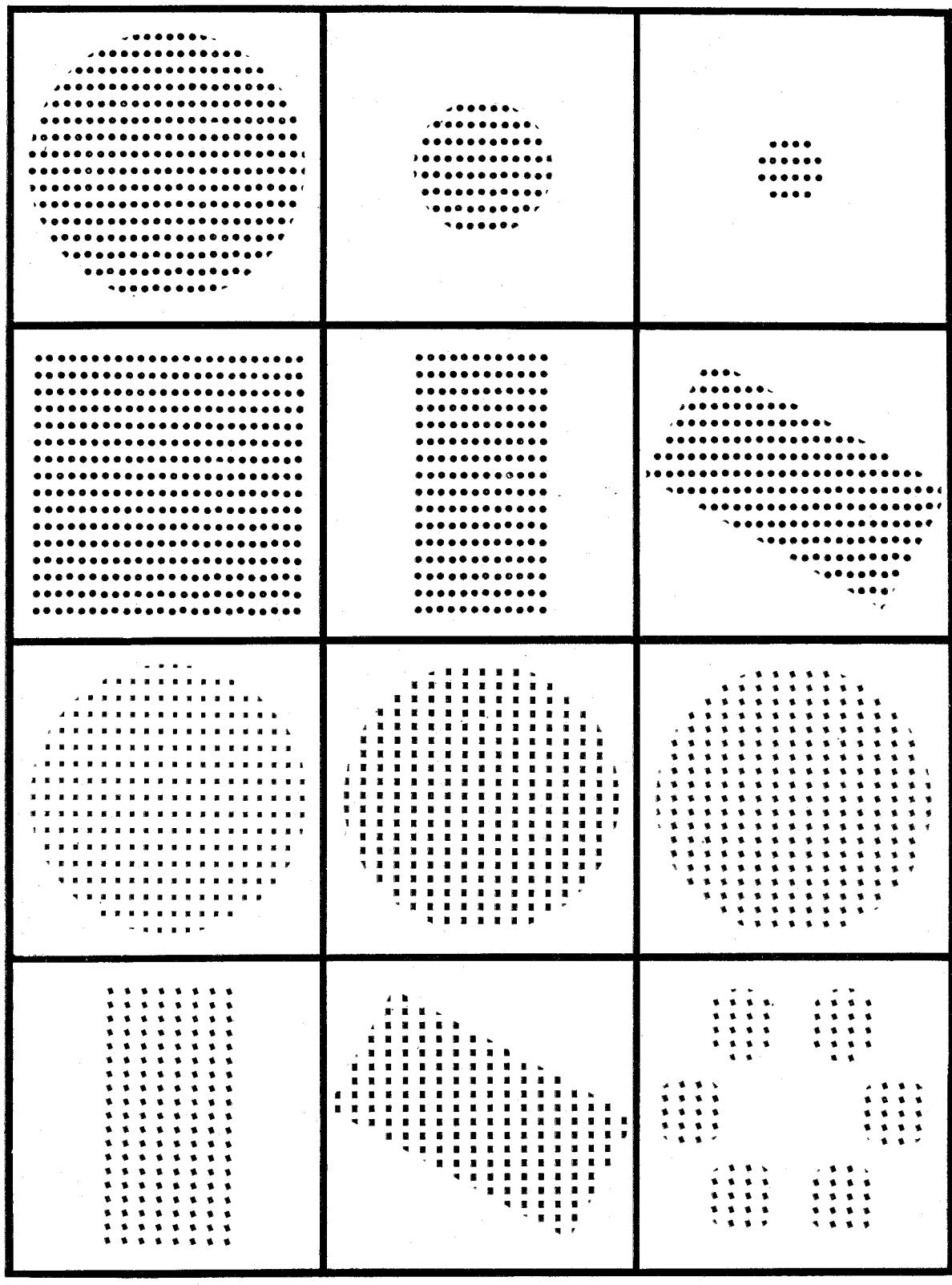


Plate 12



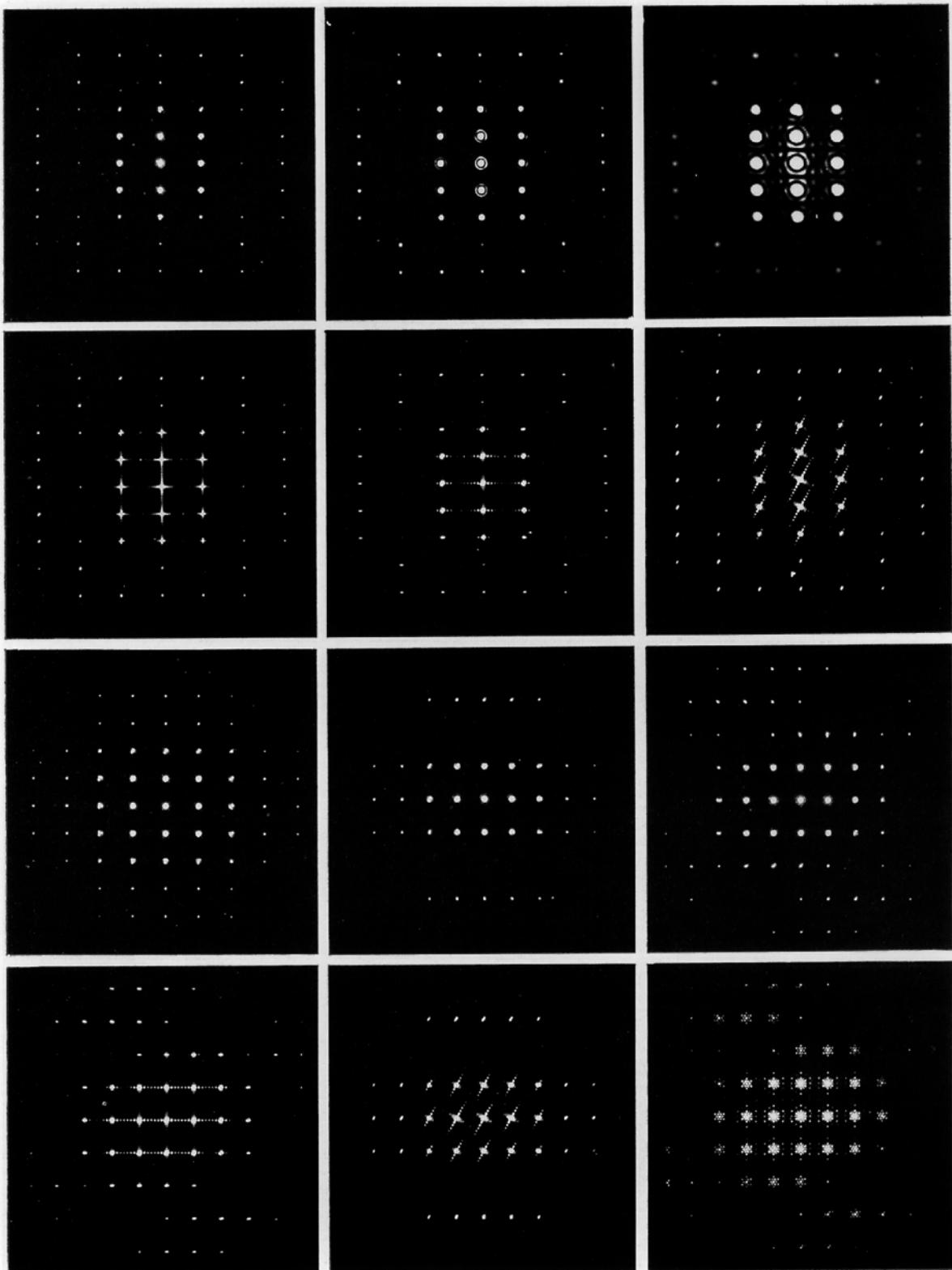
lmlmlm

Plate 13



.....

Plate 13



13-1

Plate 14

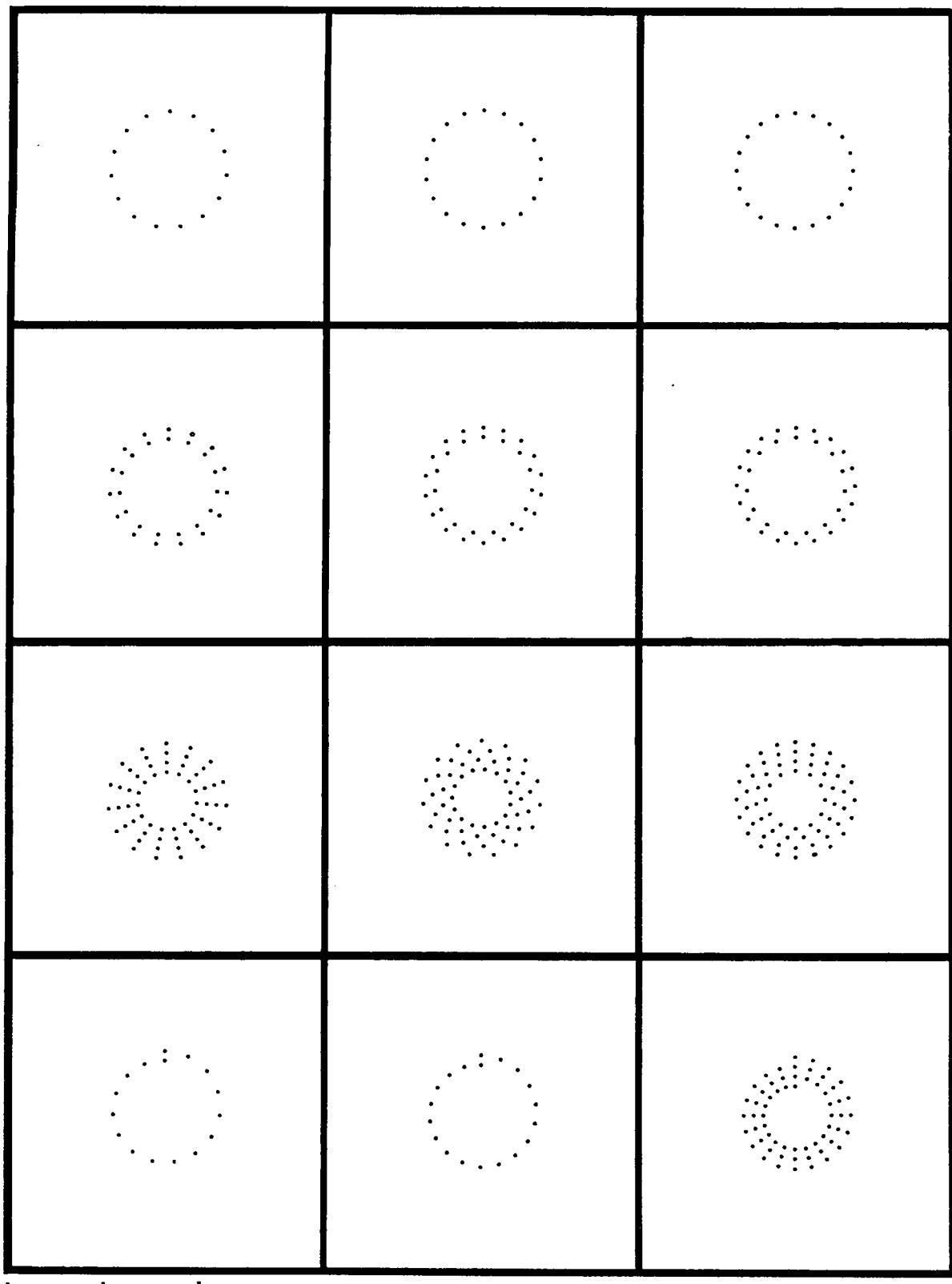


Plate 14

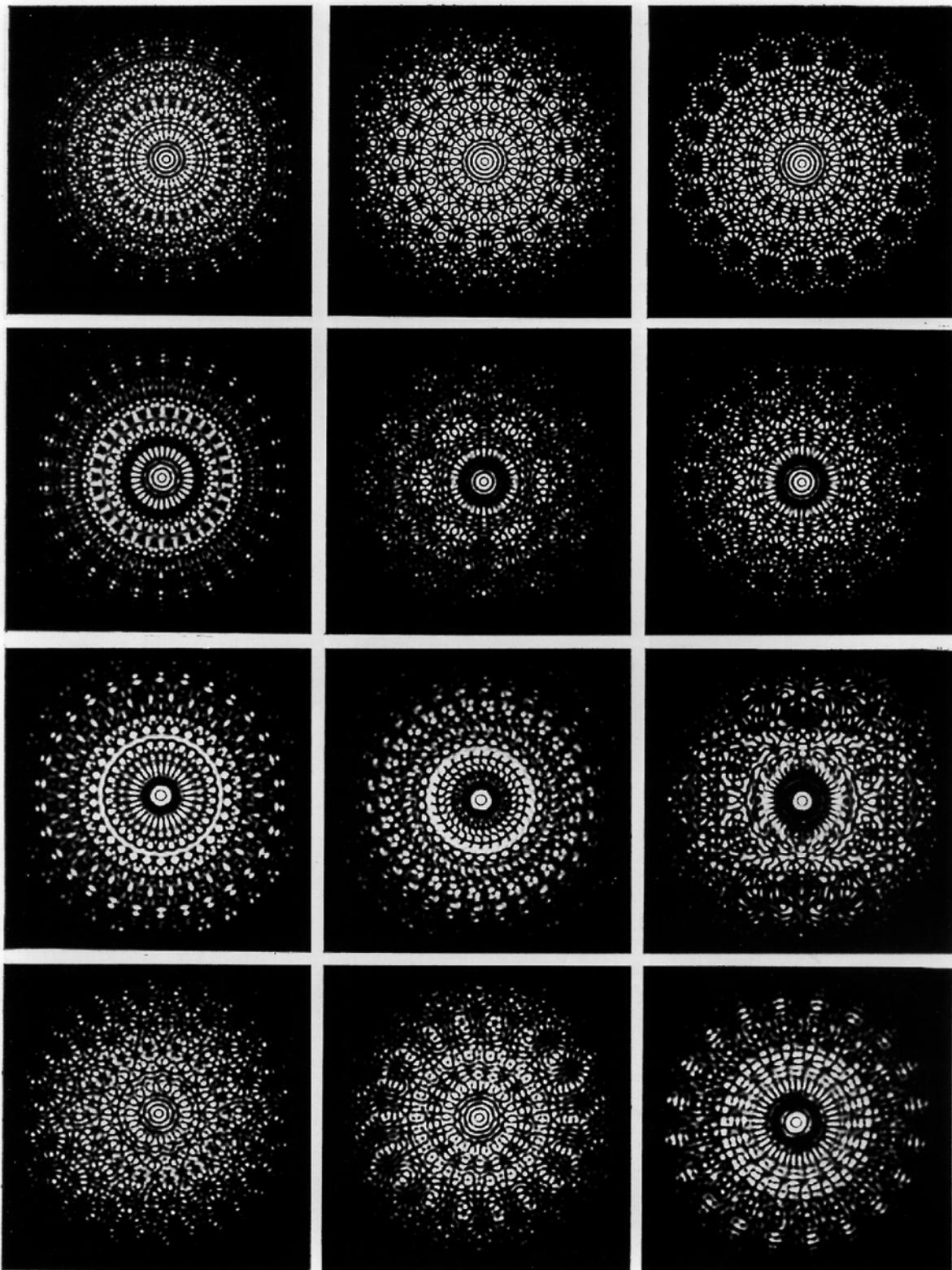
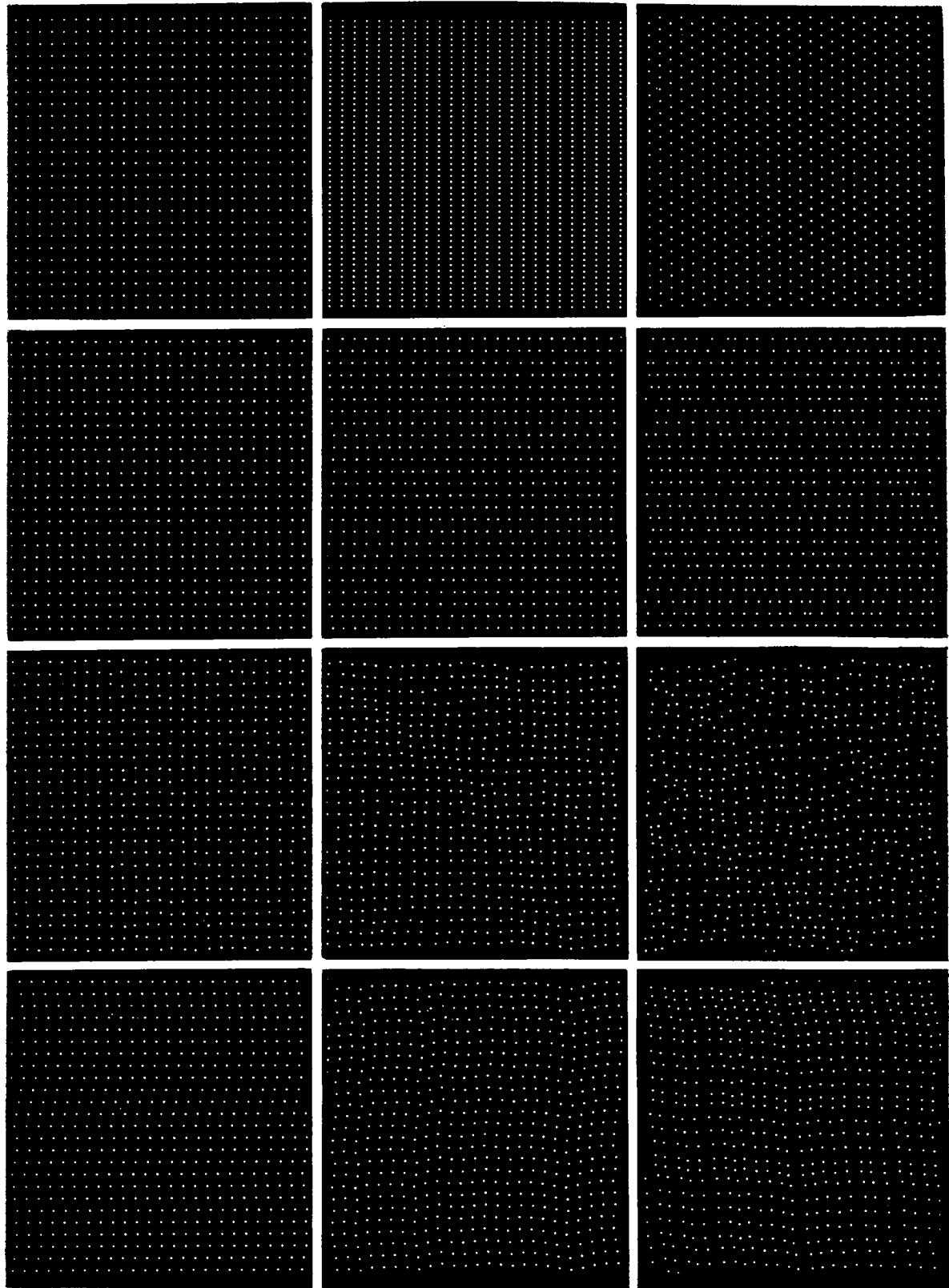


Plate 15



.....

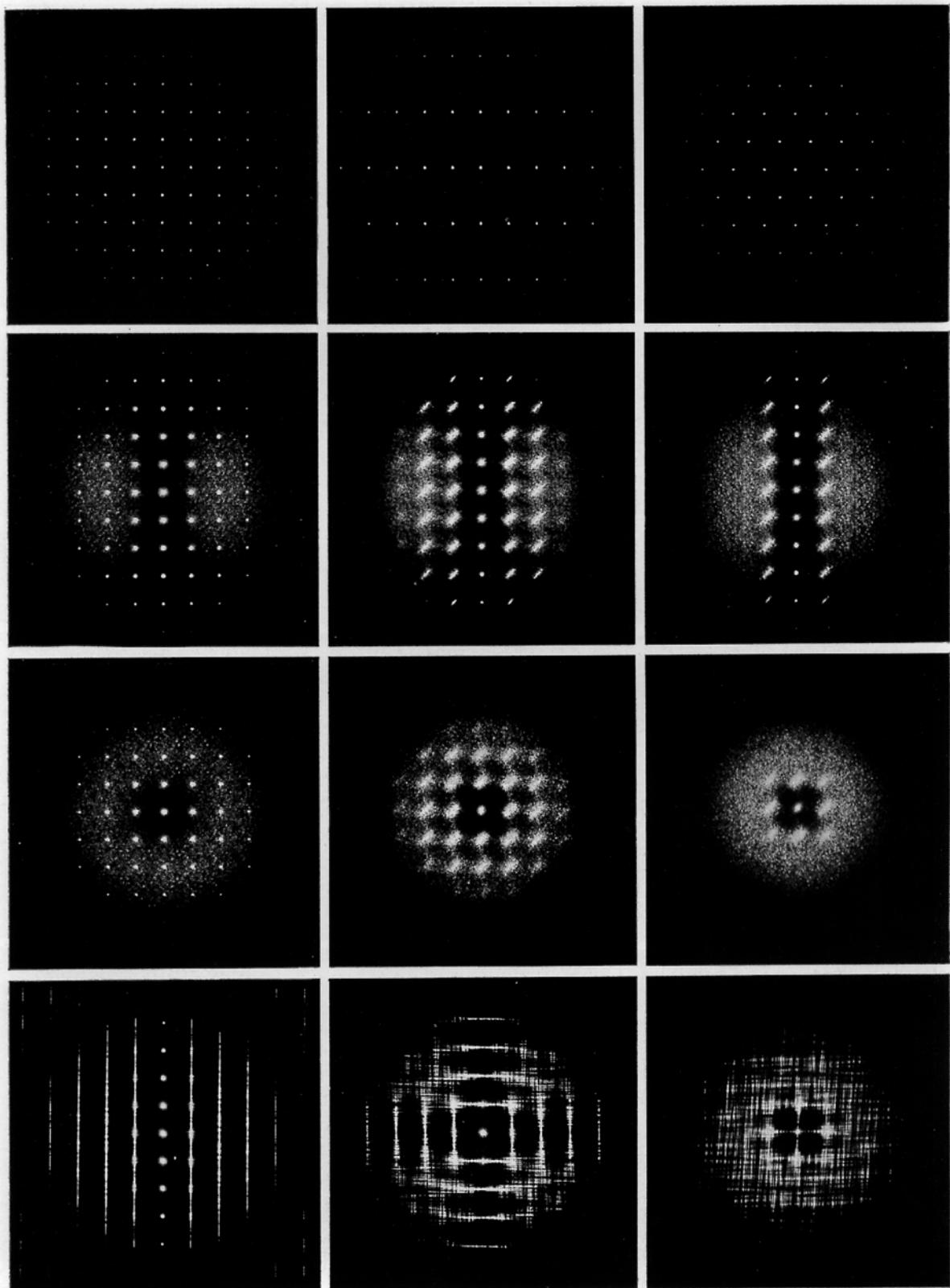
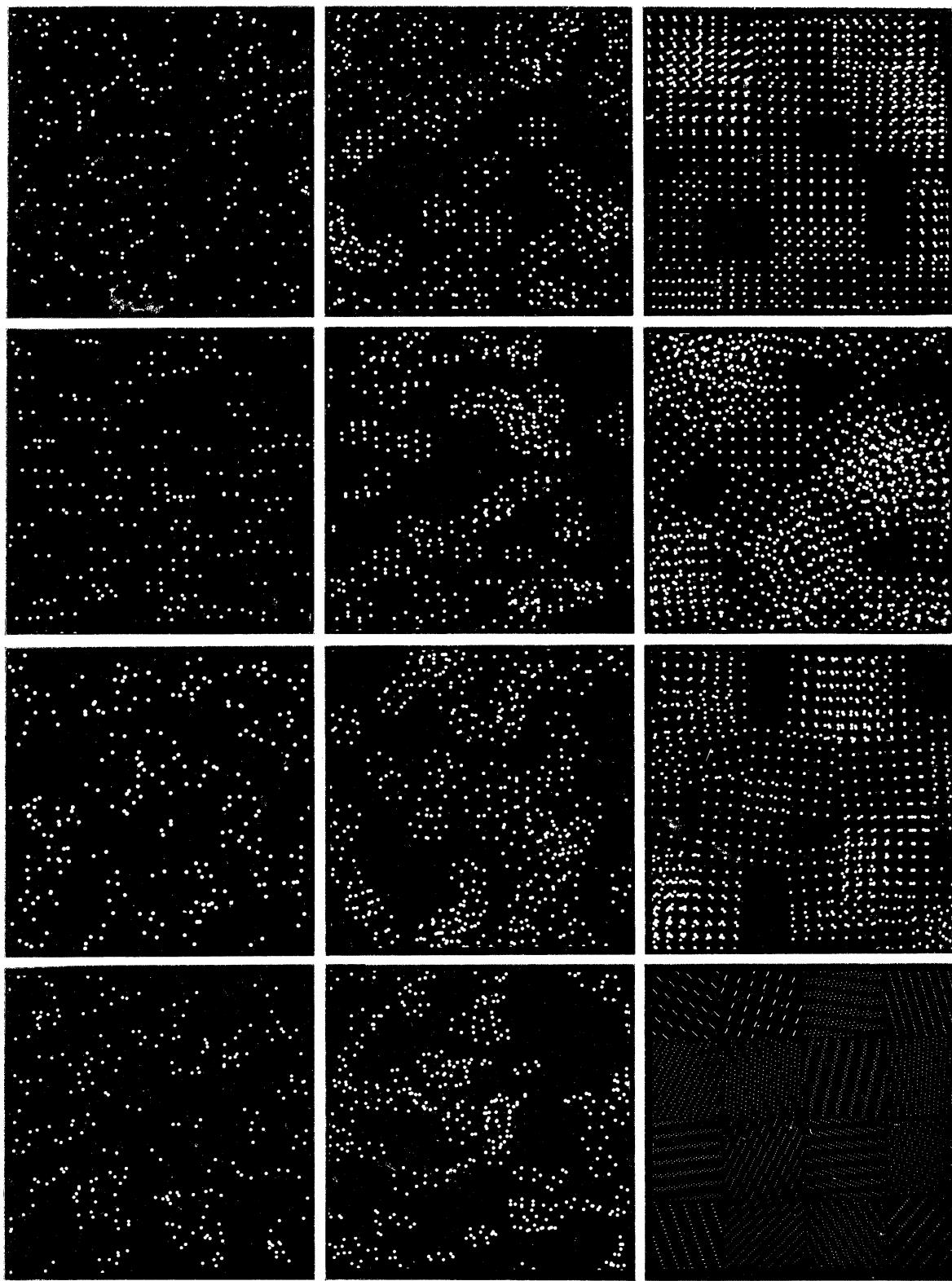


Plate 16



lmlmlml

Plate 16

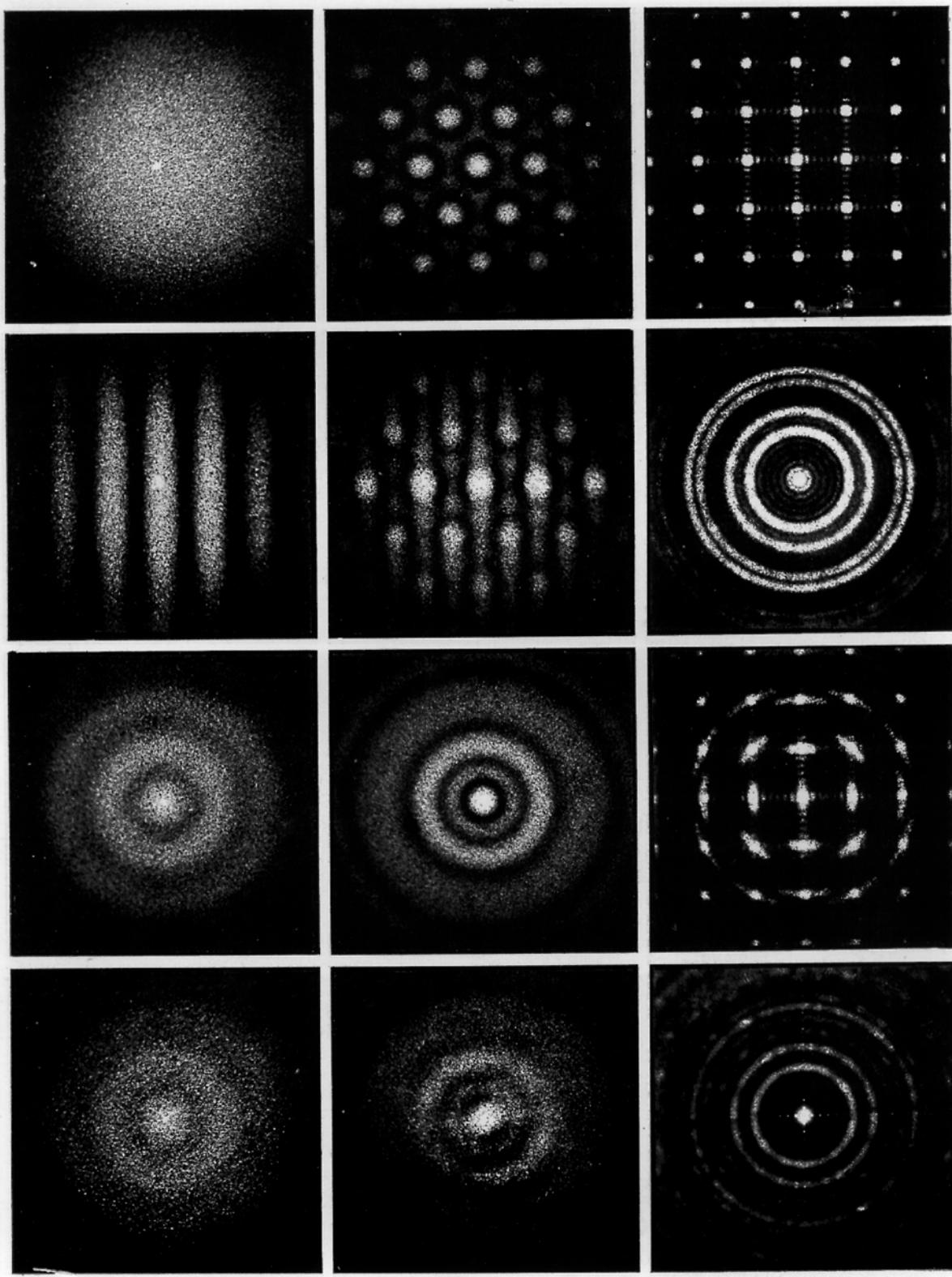
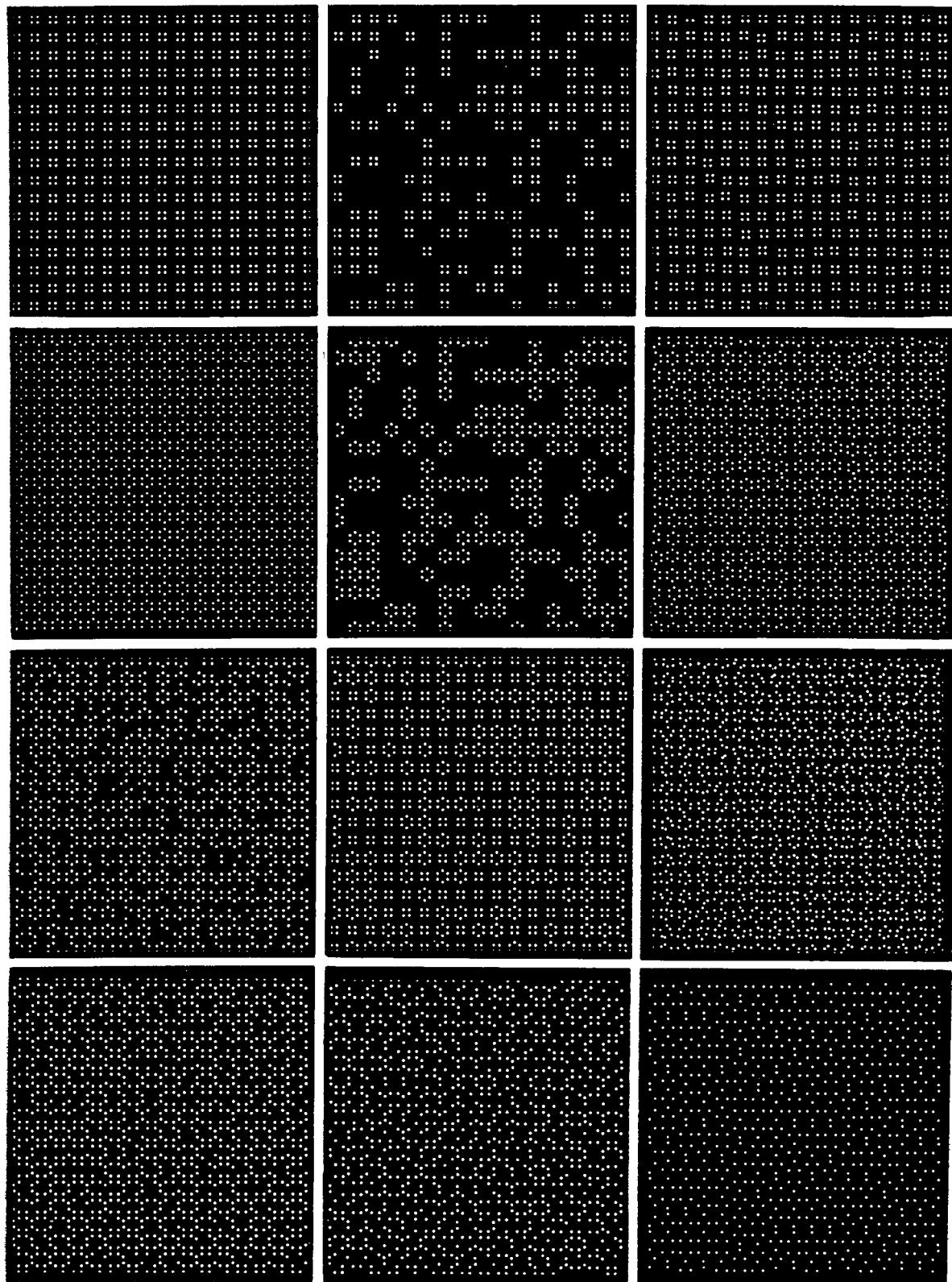


Plate 17



⠠⠠⠠⠠⠠⠠⠠

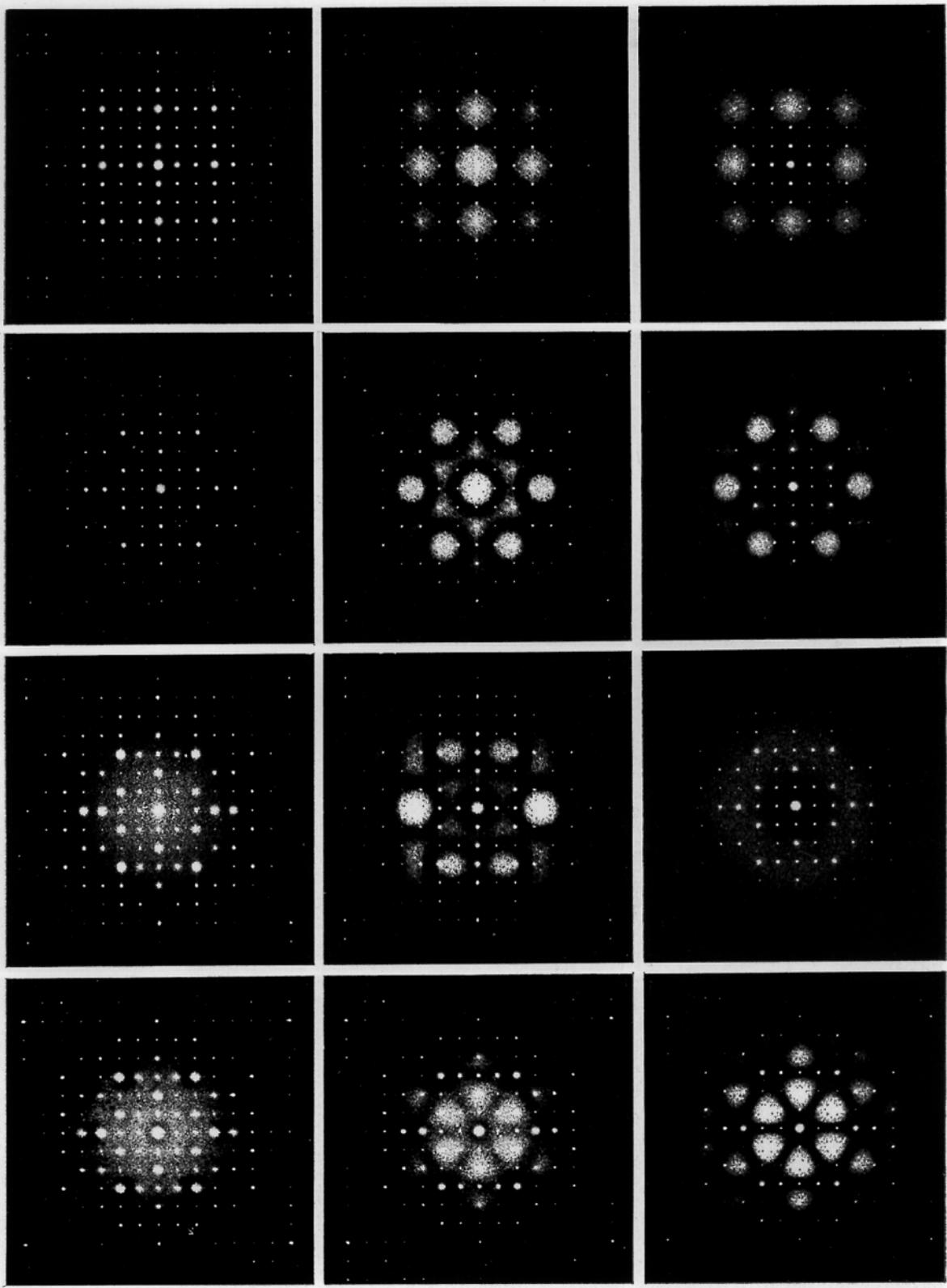
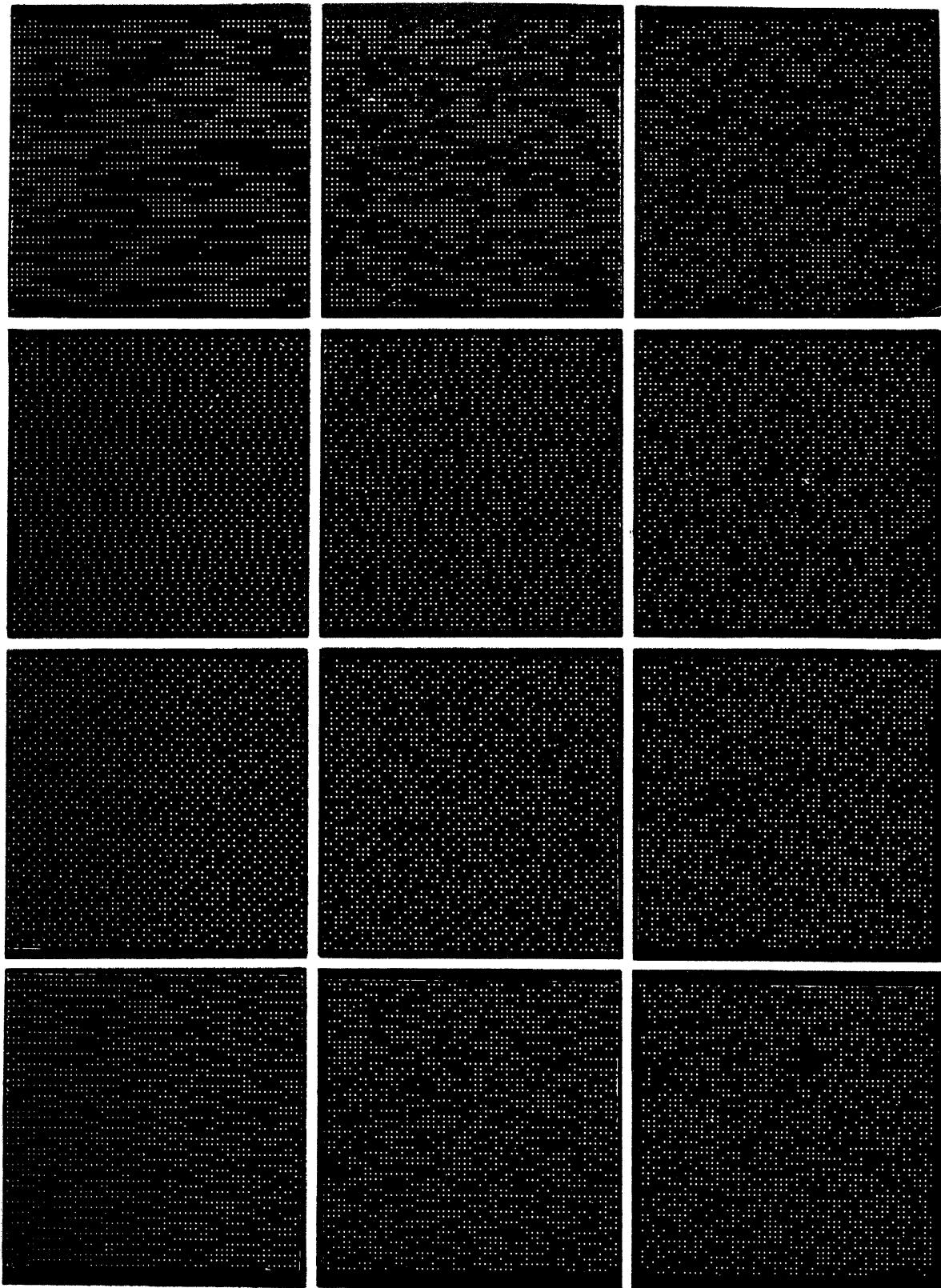
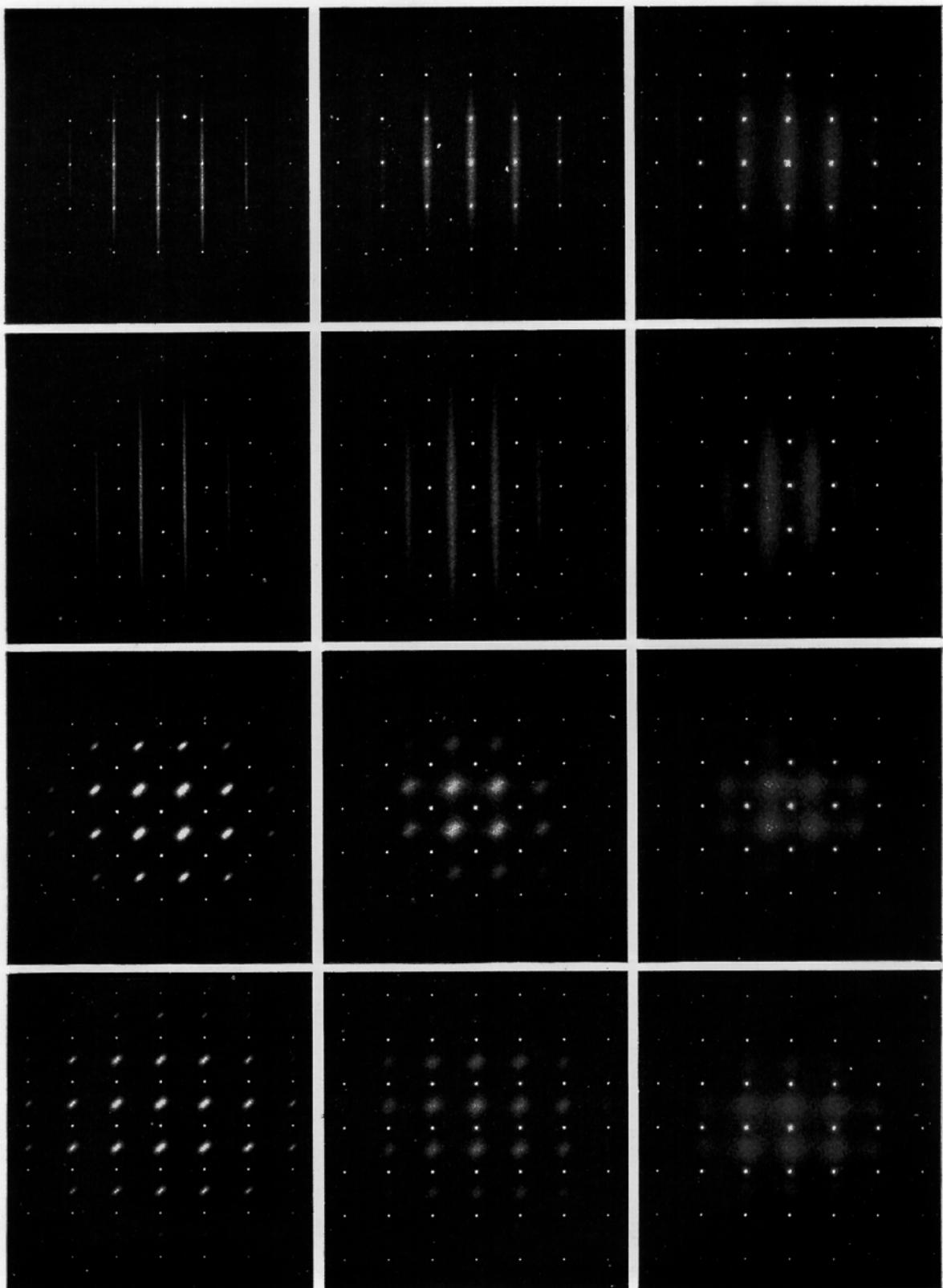


Plate 18



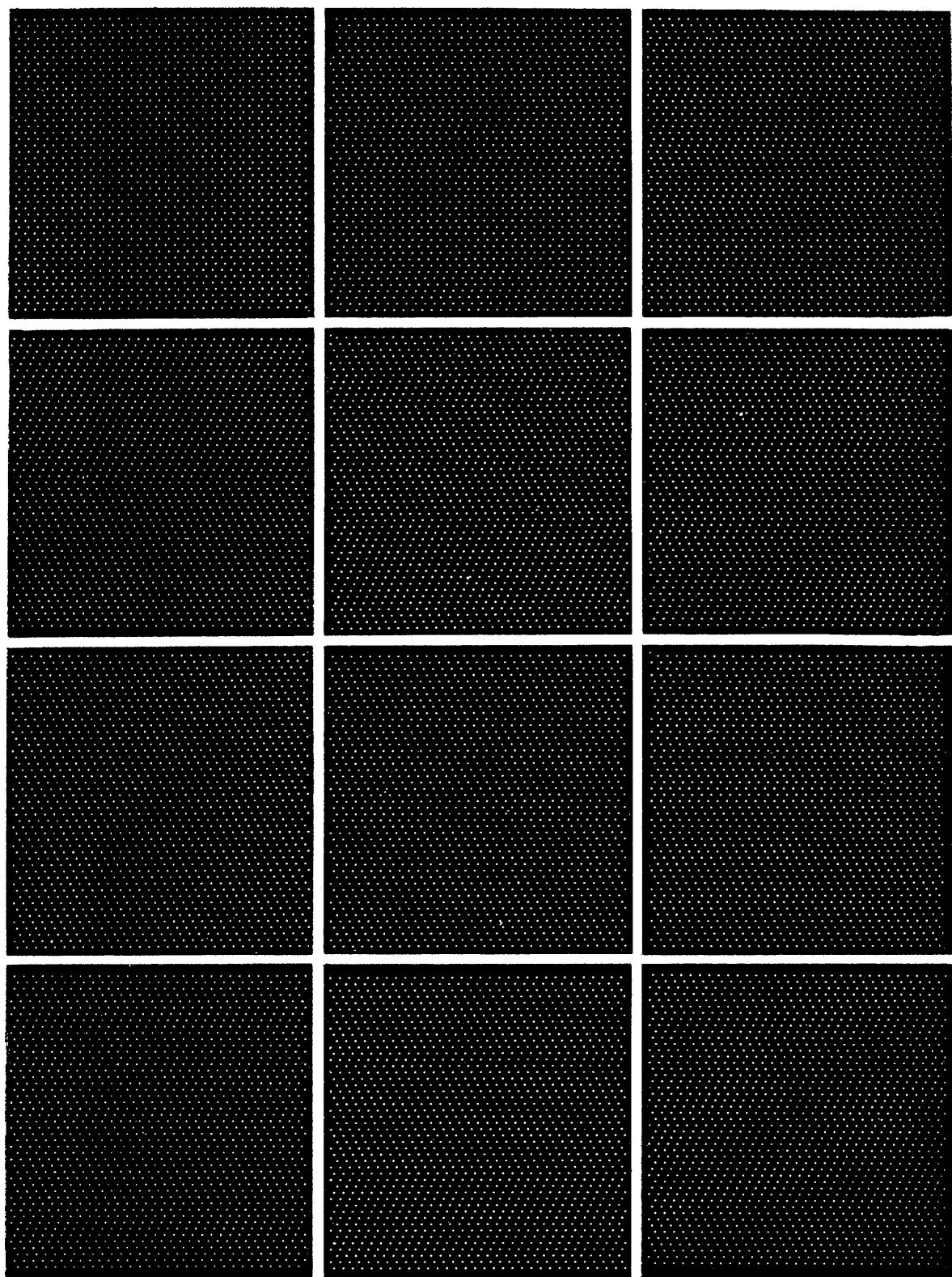
lindblad

Plate 18



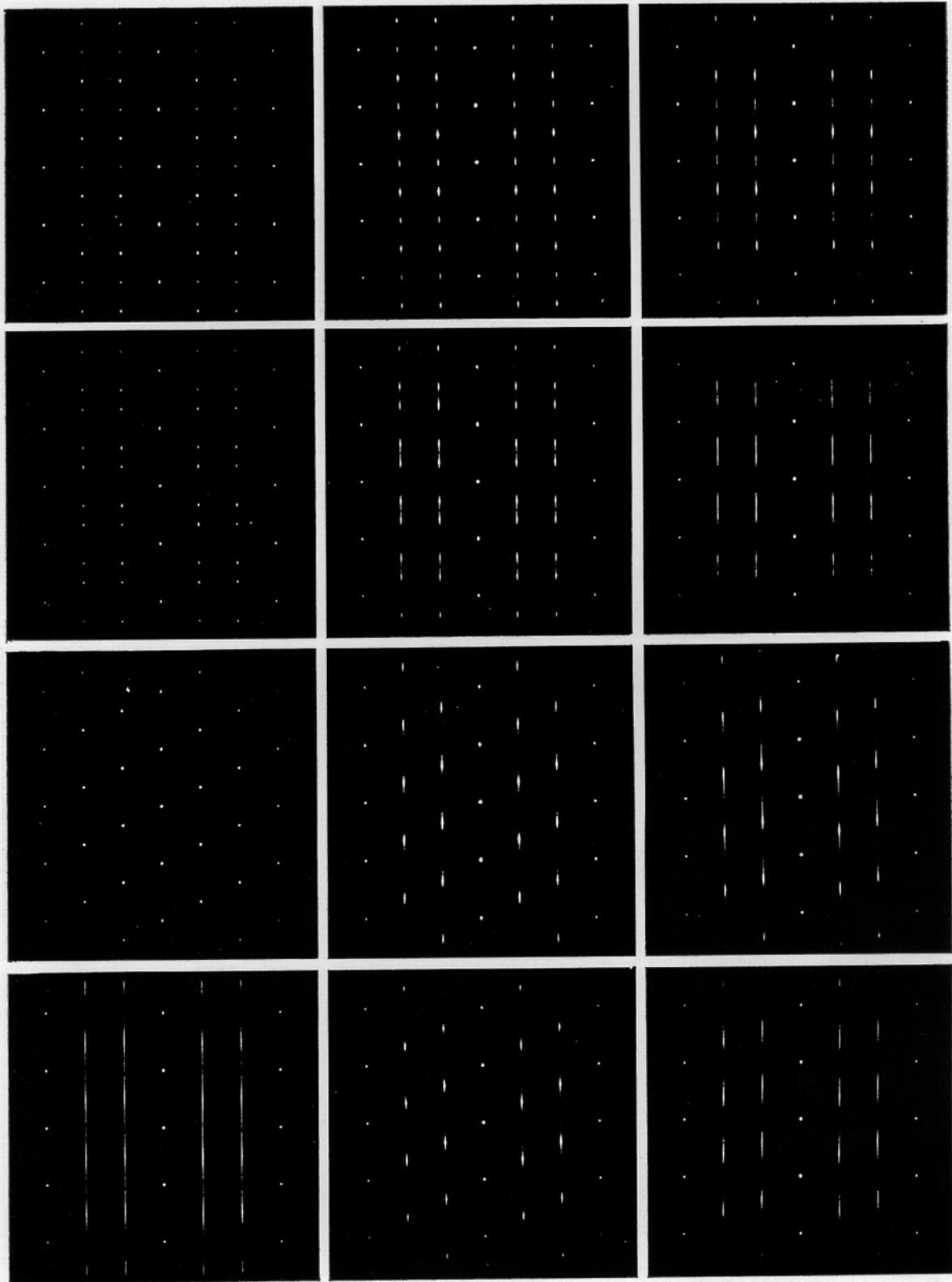
11111

Plate 19



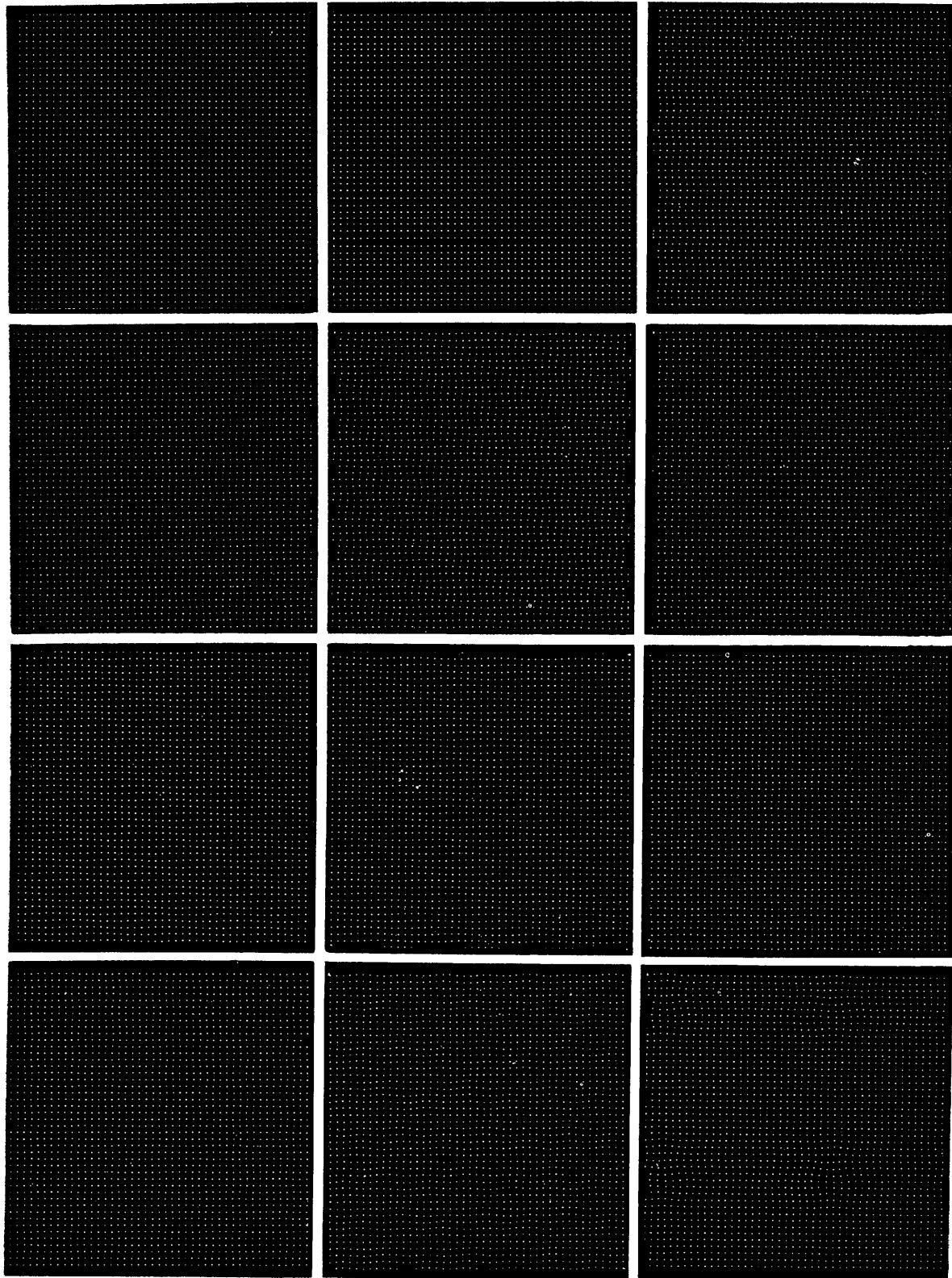
frontend

Plate 19



1 2 3 4 5 6

Plate 20



bookl

Plate 20

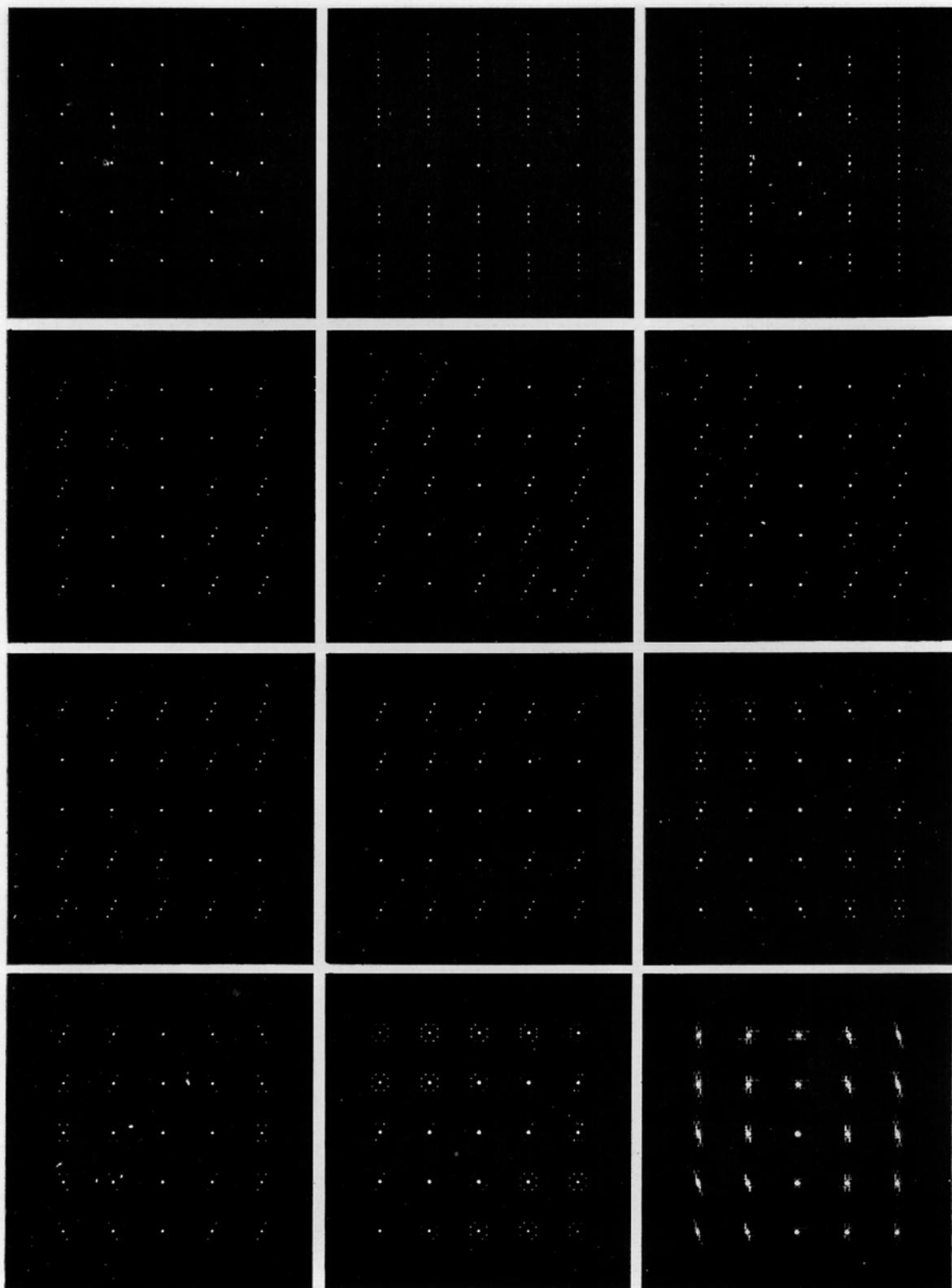


Plate 21

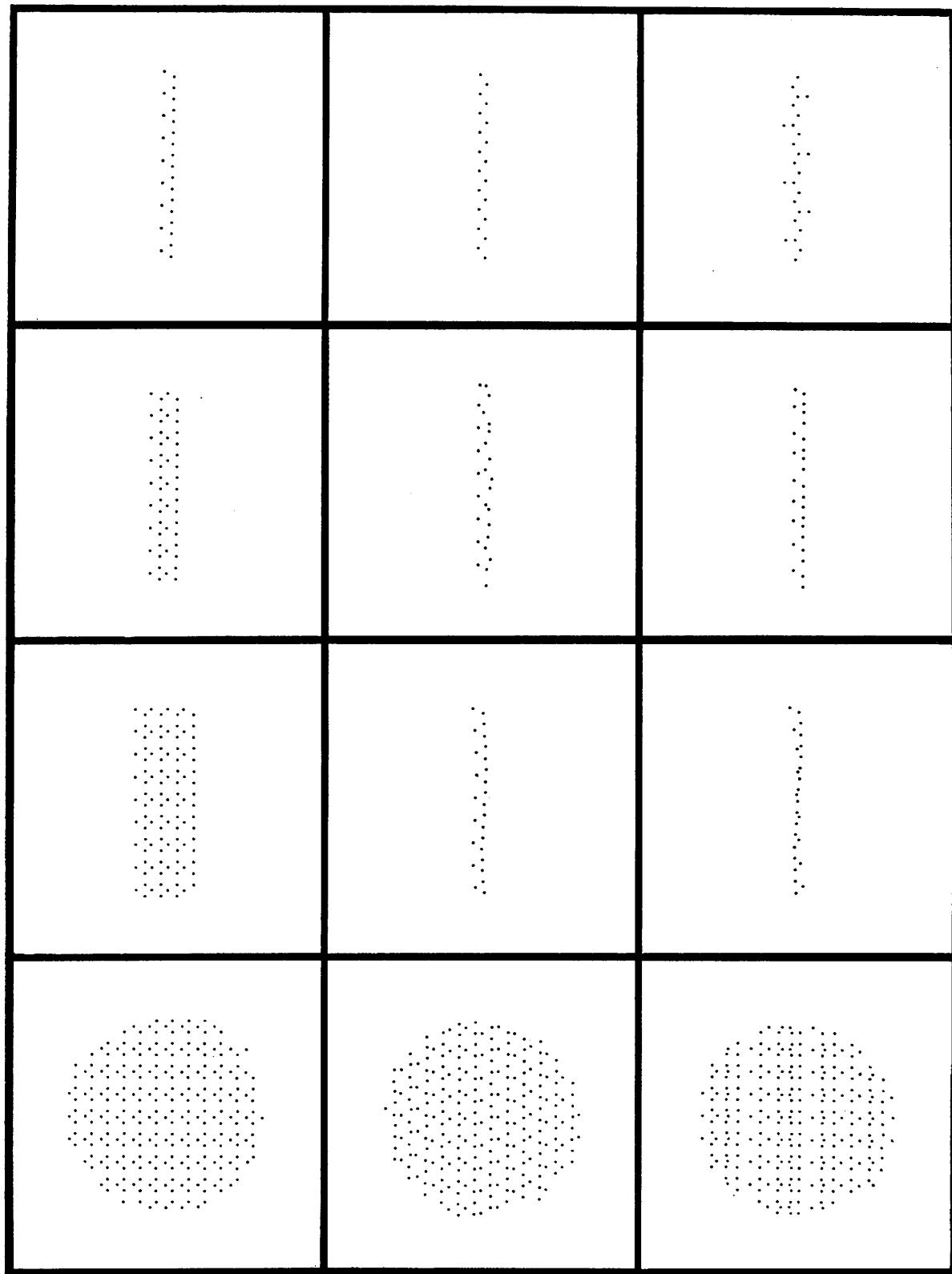
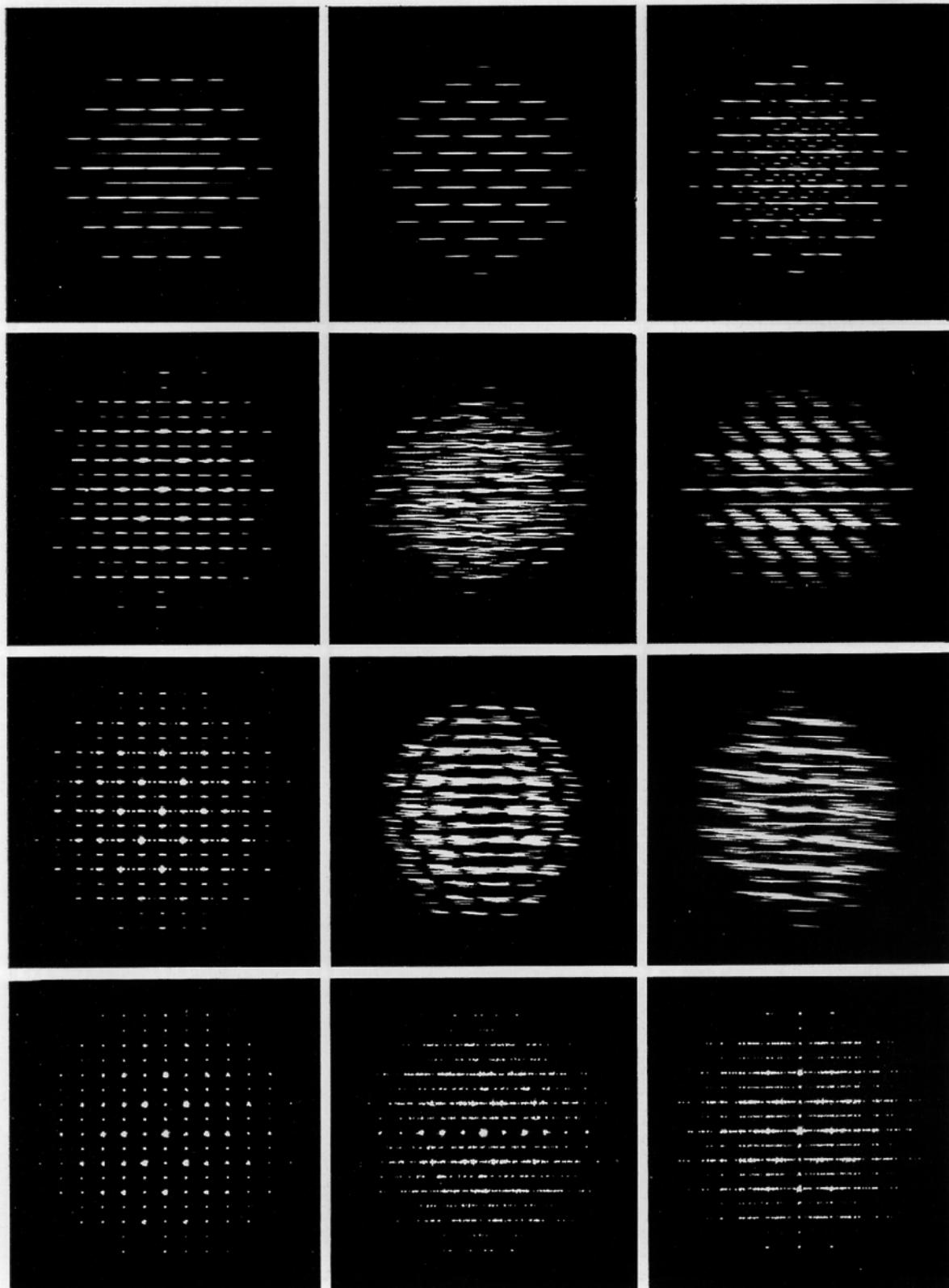


Plate 21



l l l l l l

Plate 22

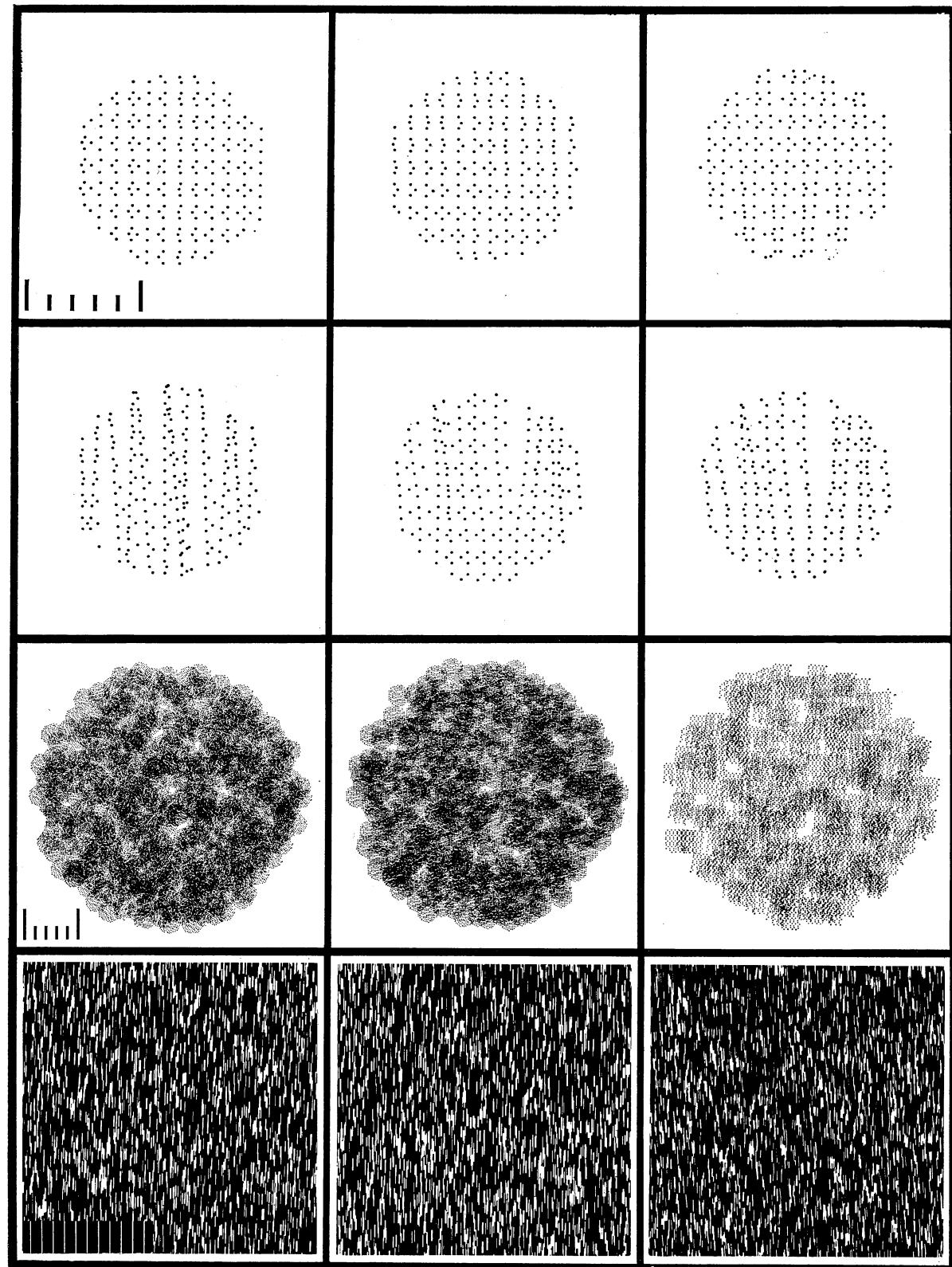


Plate 22

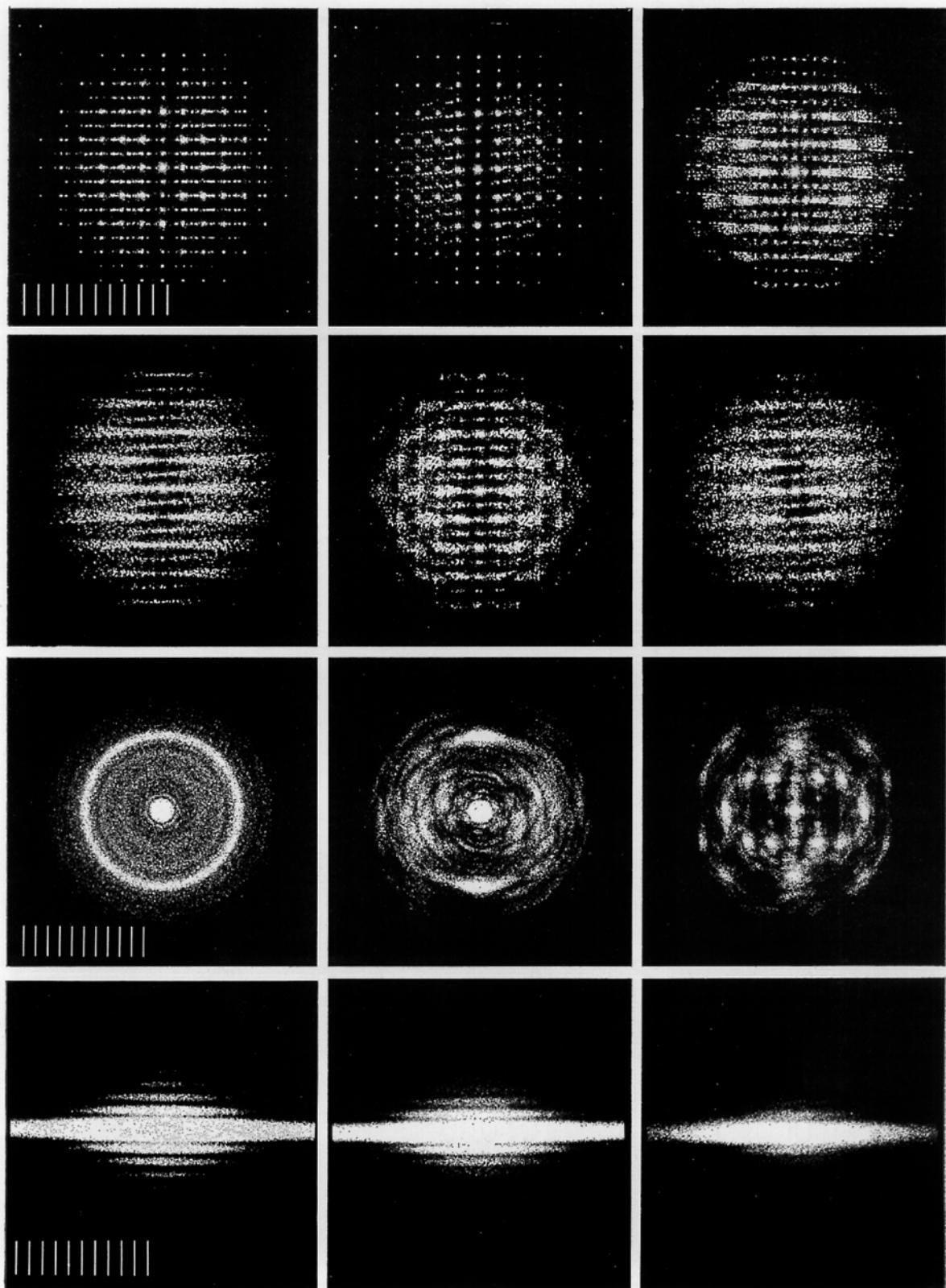


Plate 23

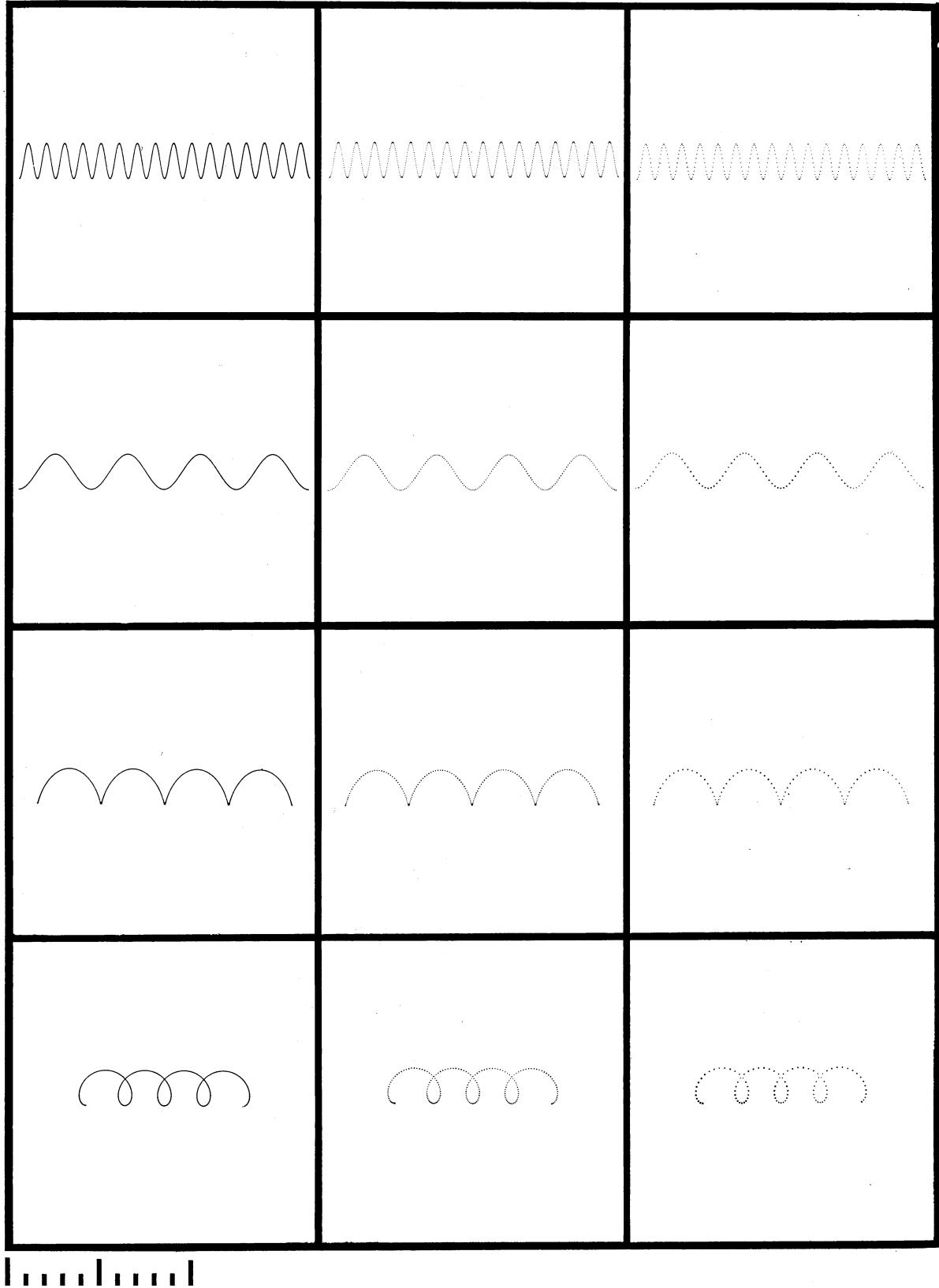
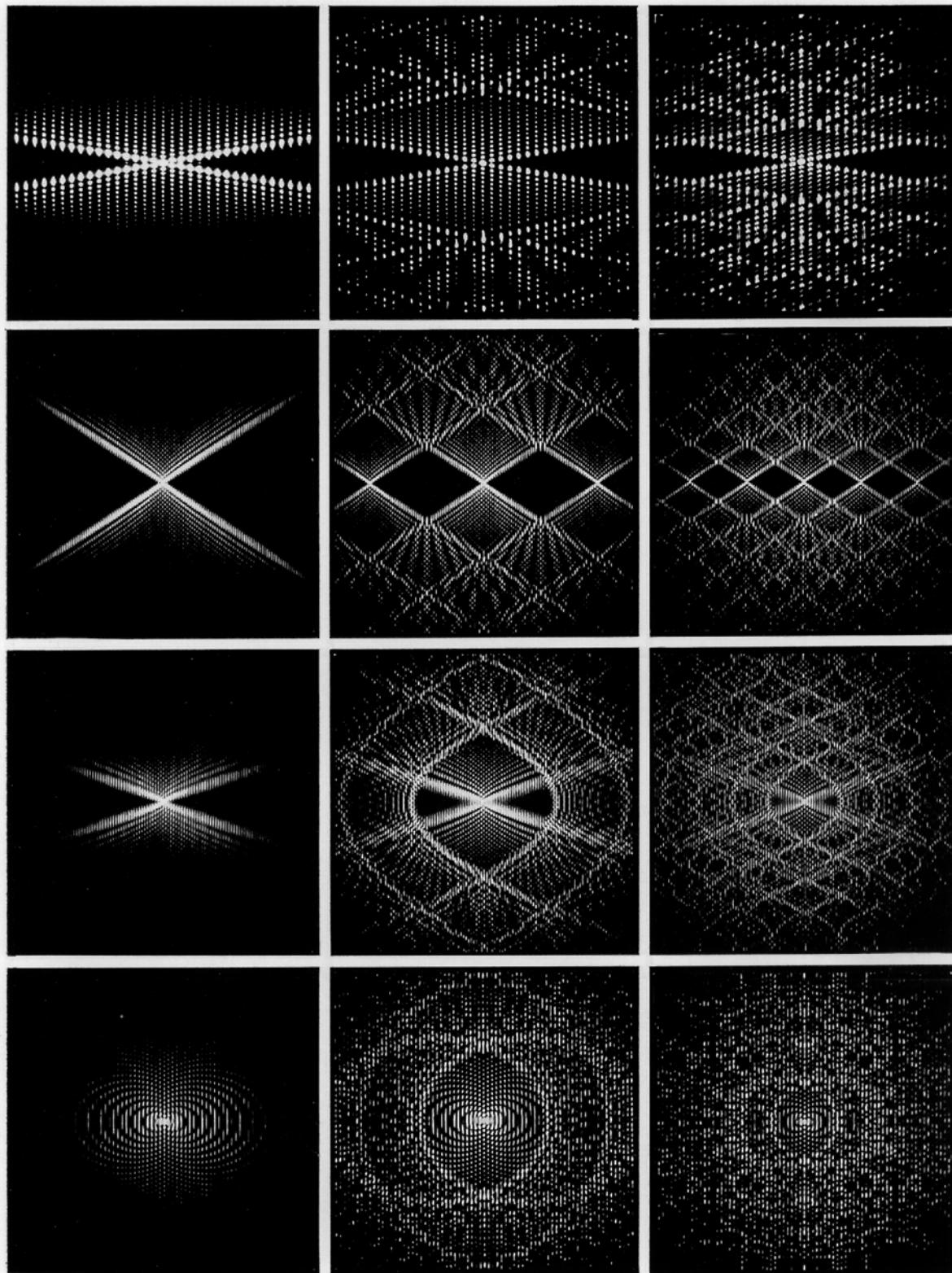


Plate 23



lmlmlm

Plate 24

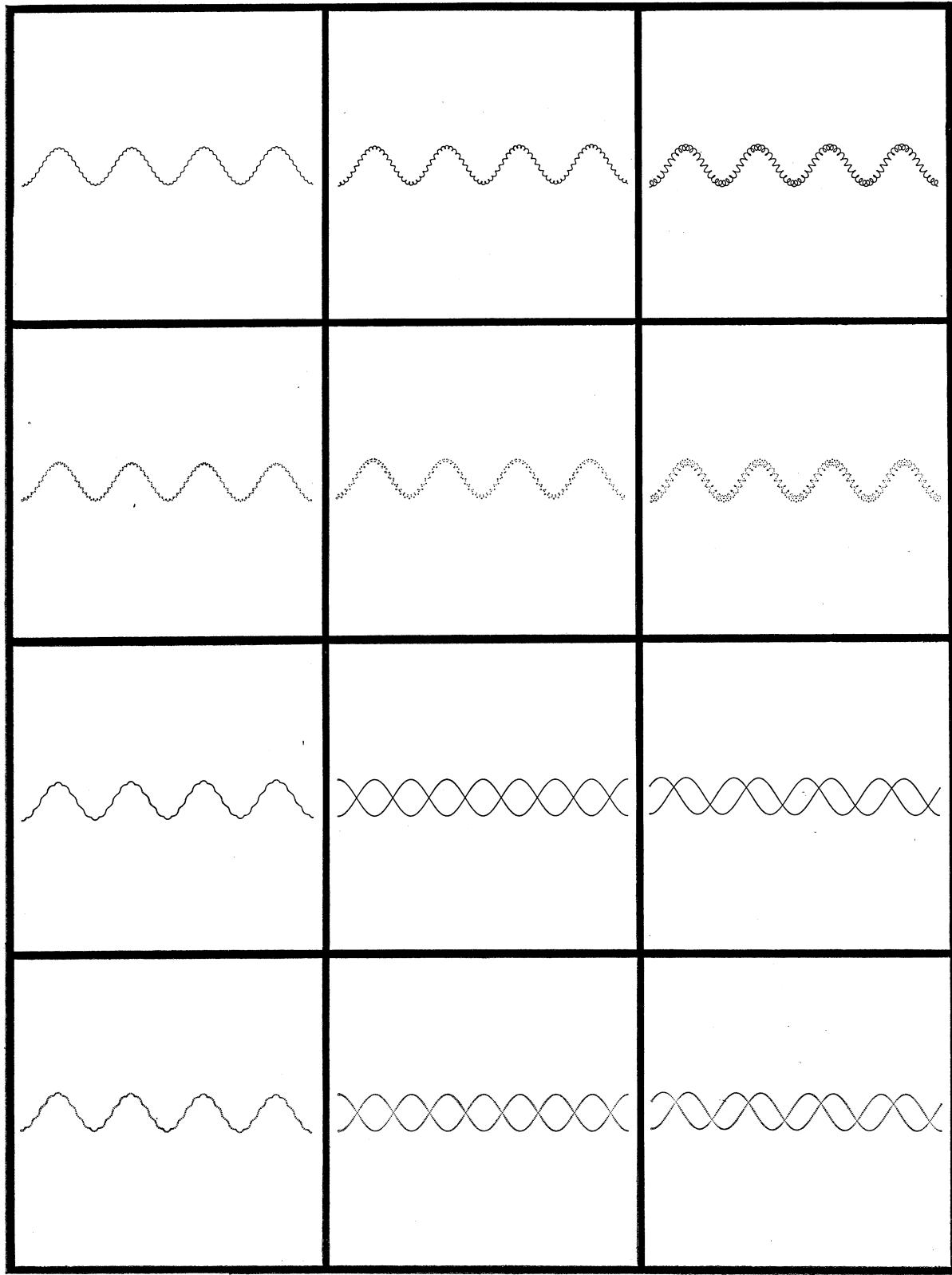
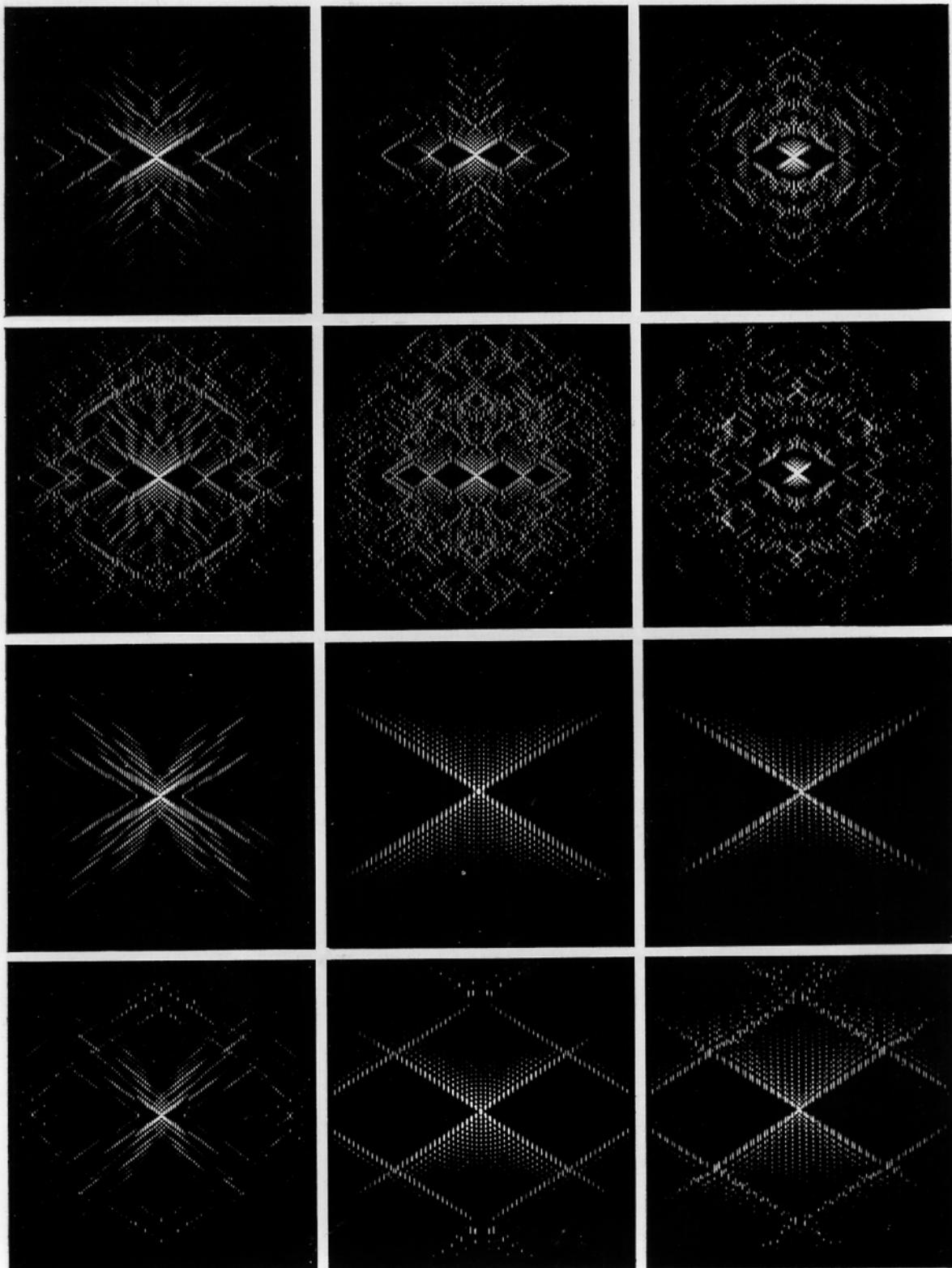


Plate 24



Individ

Individ

Plate 25

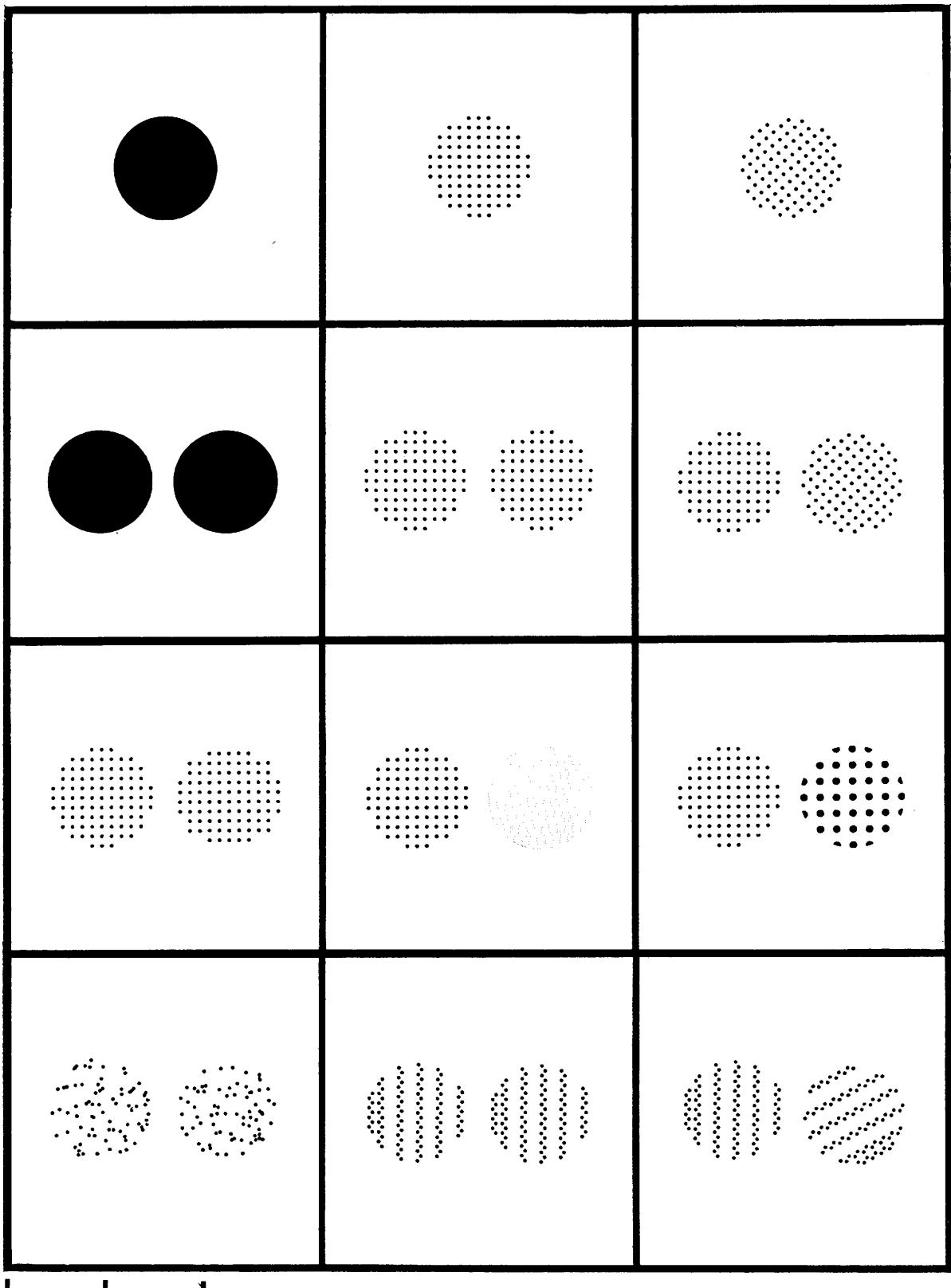


Plate 25

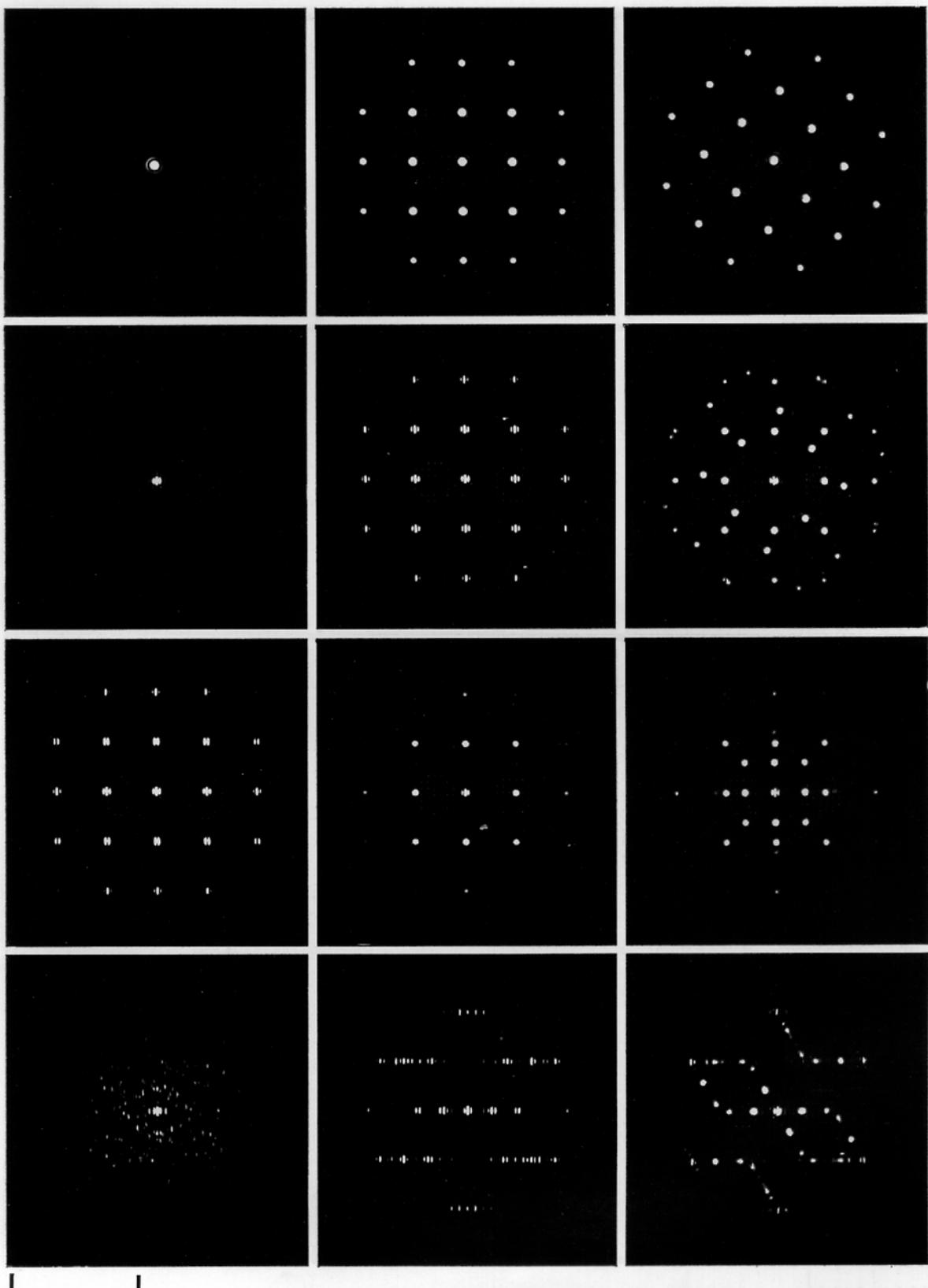
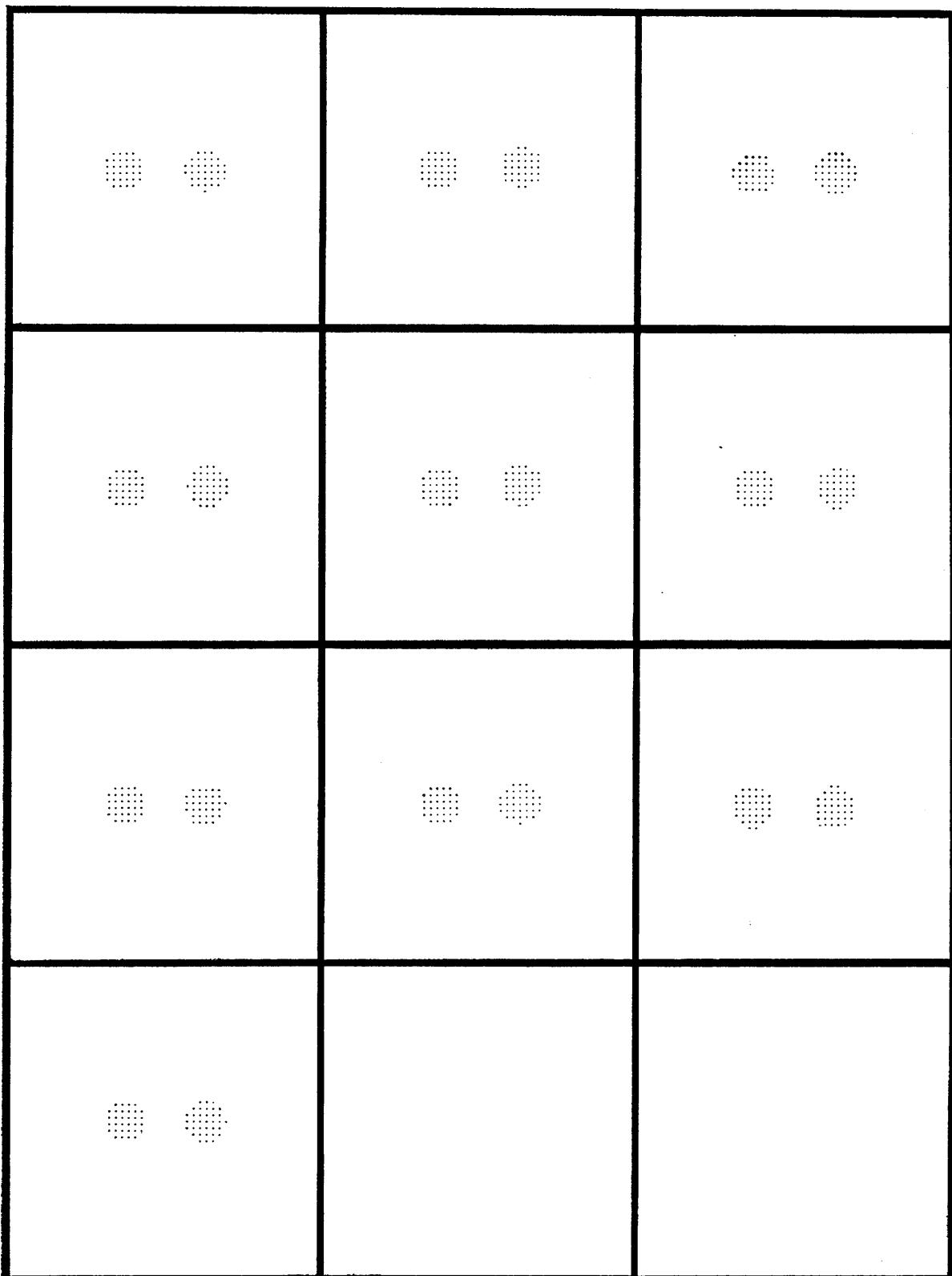
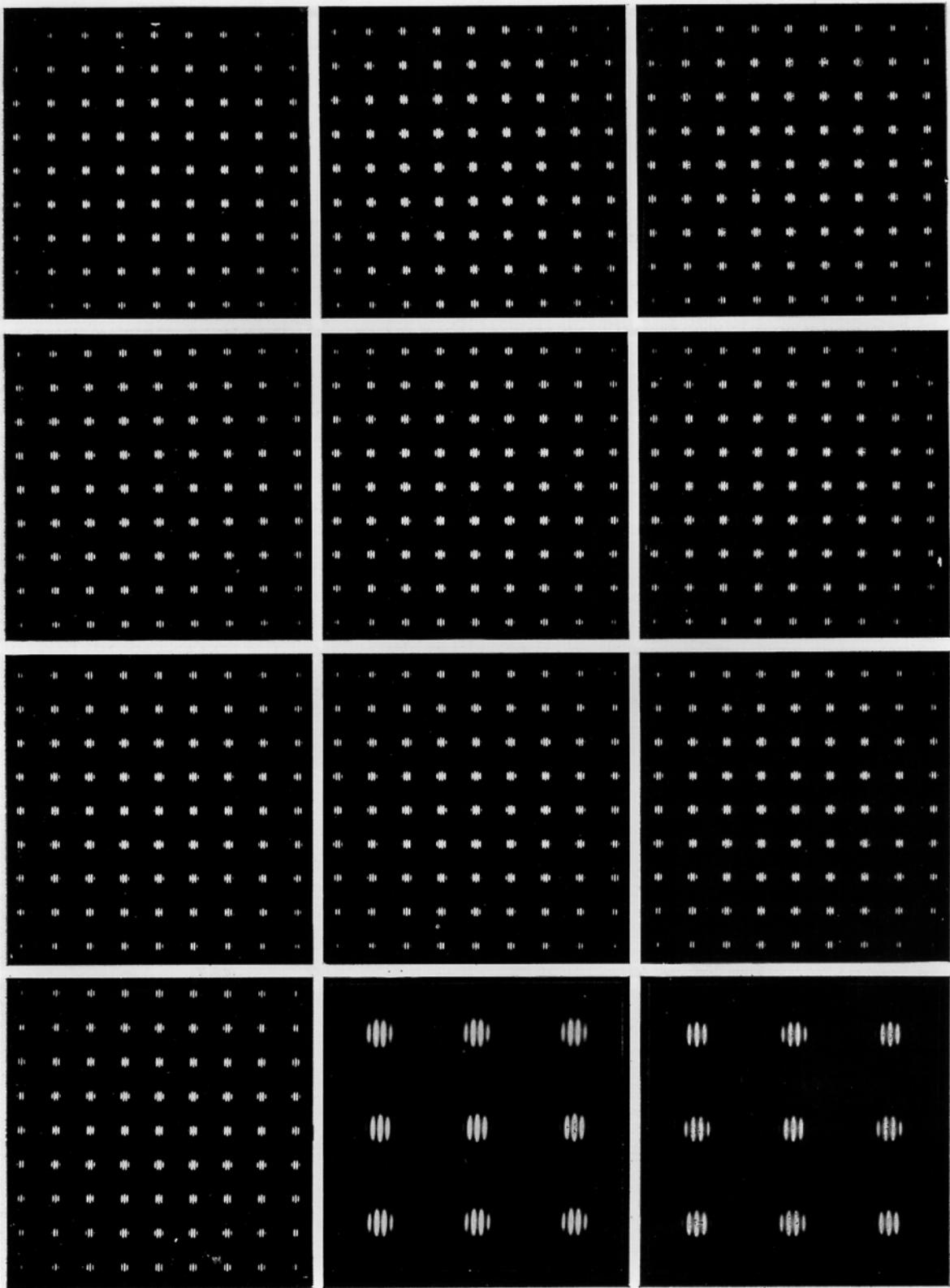


Plate 26



lmlml

Plate 26



1 2 3 4 5 6

Plate 27

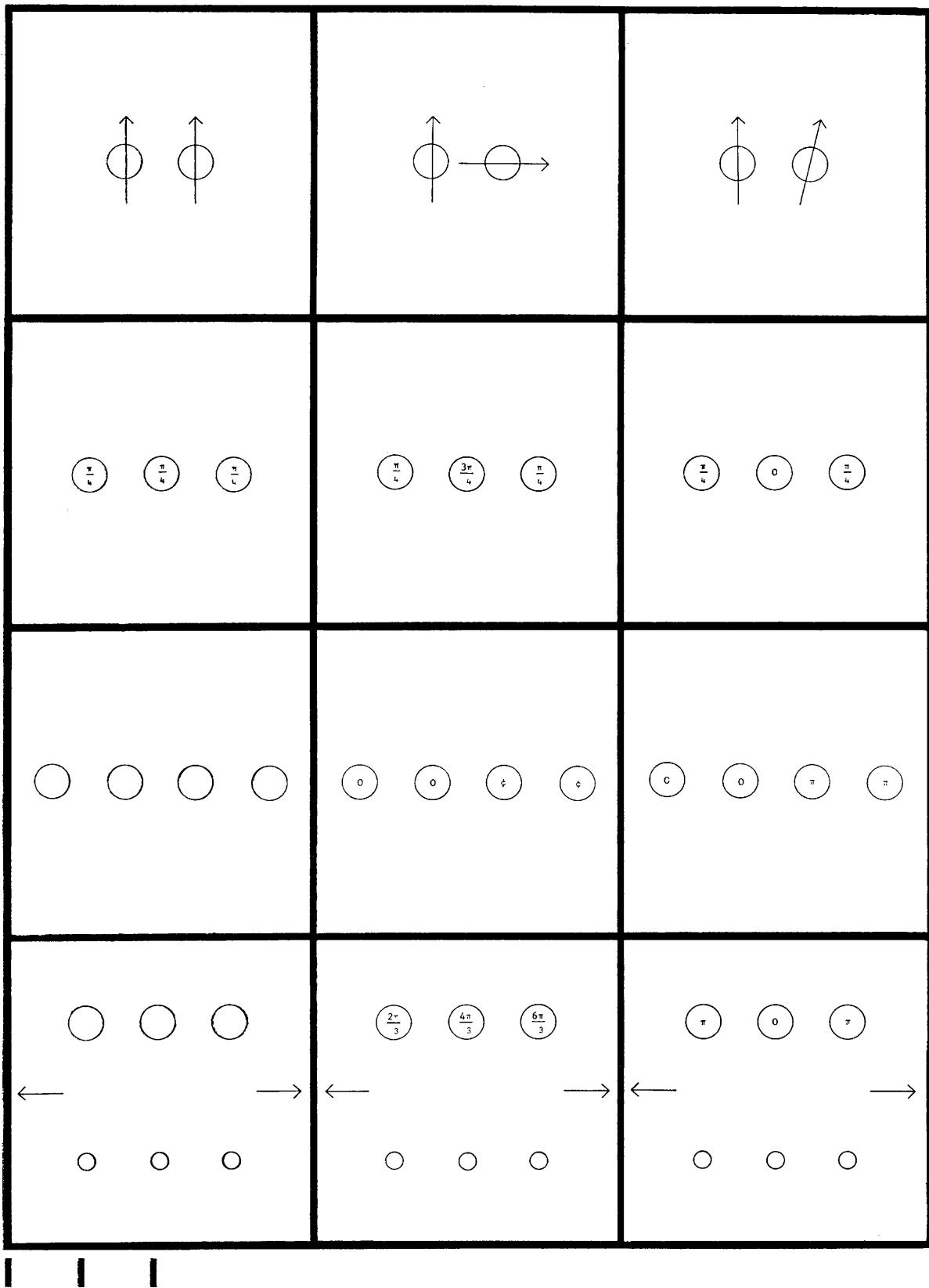


Plate 27

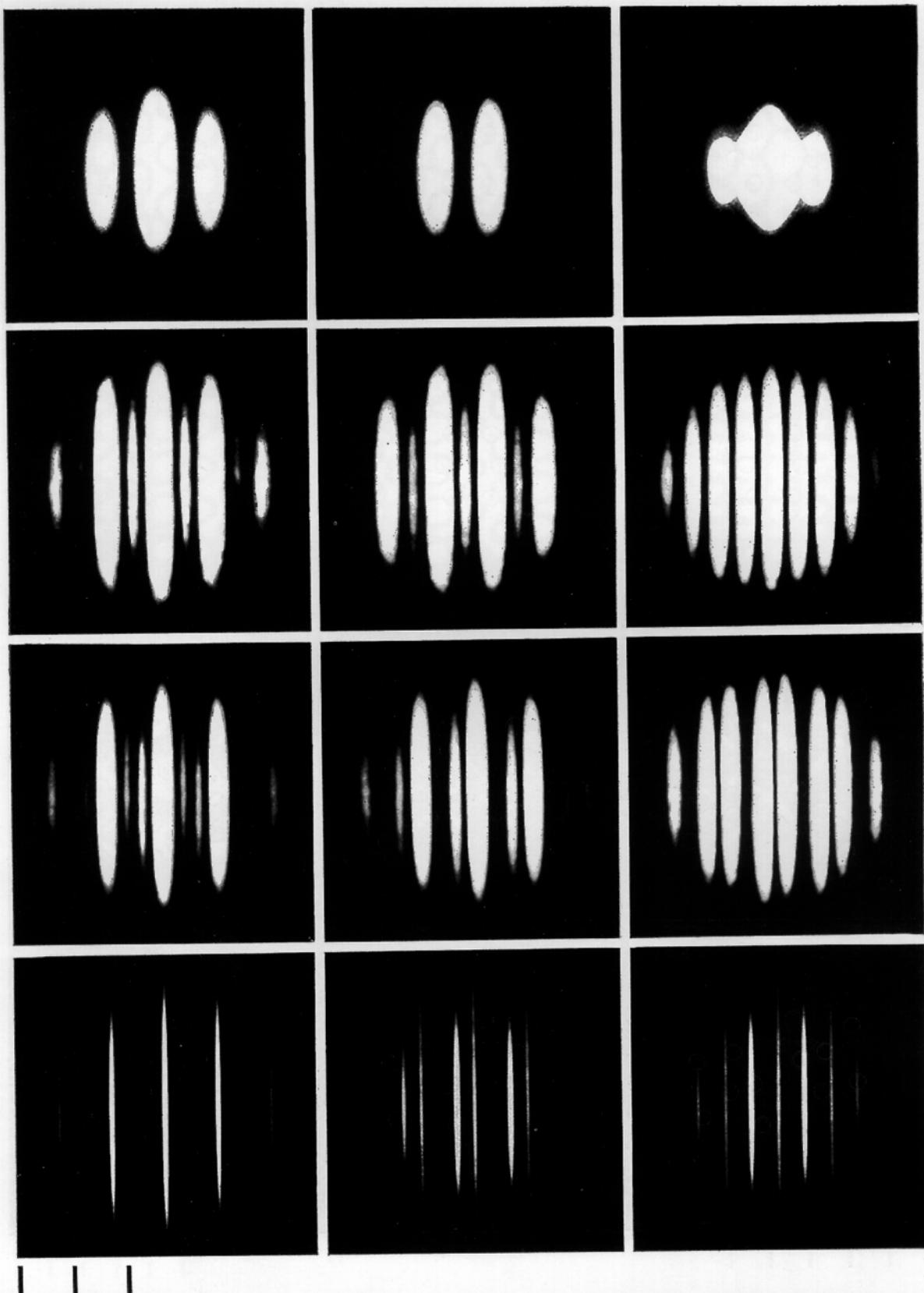


Plate 28

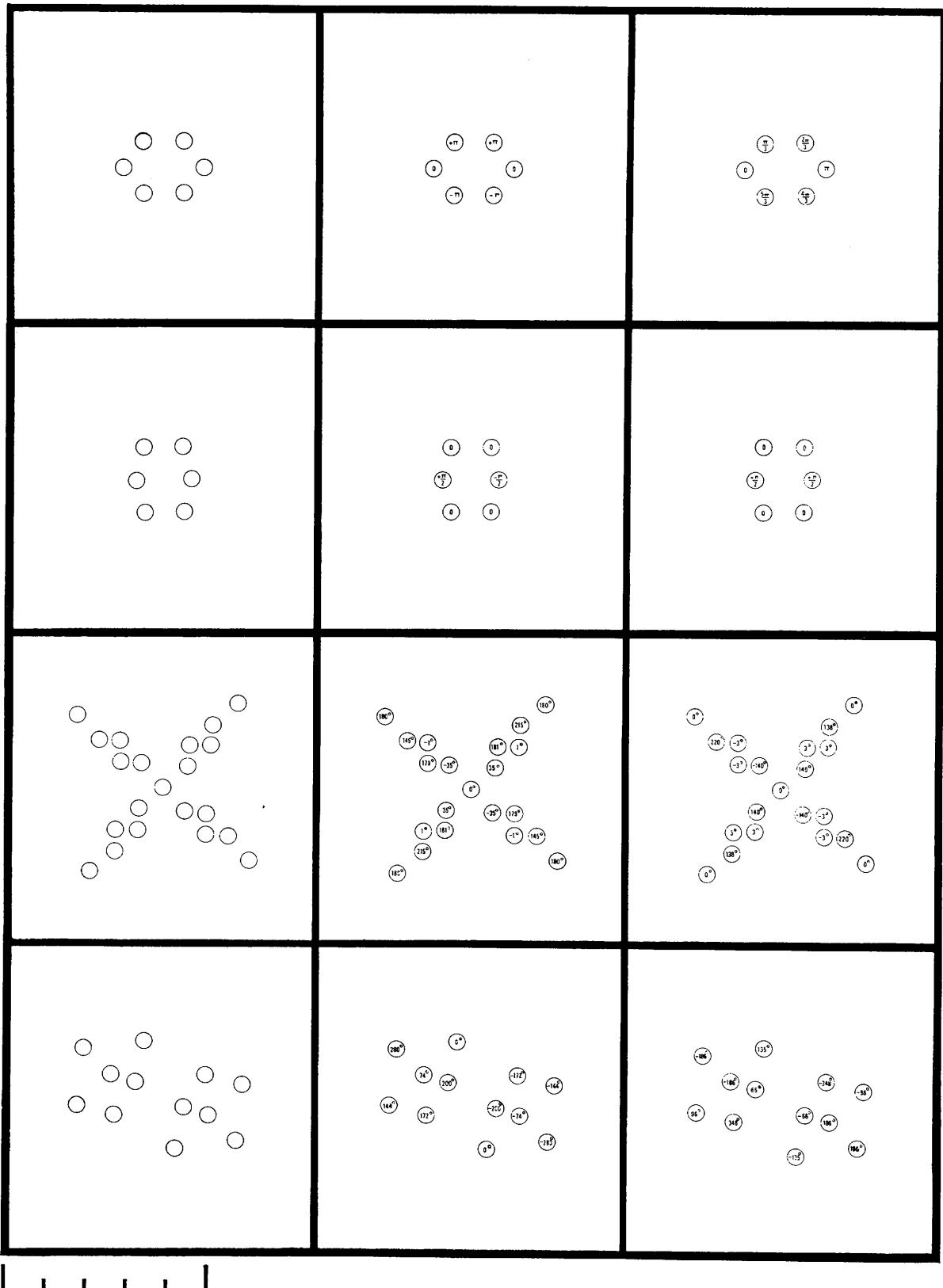


Plate 28

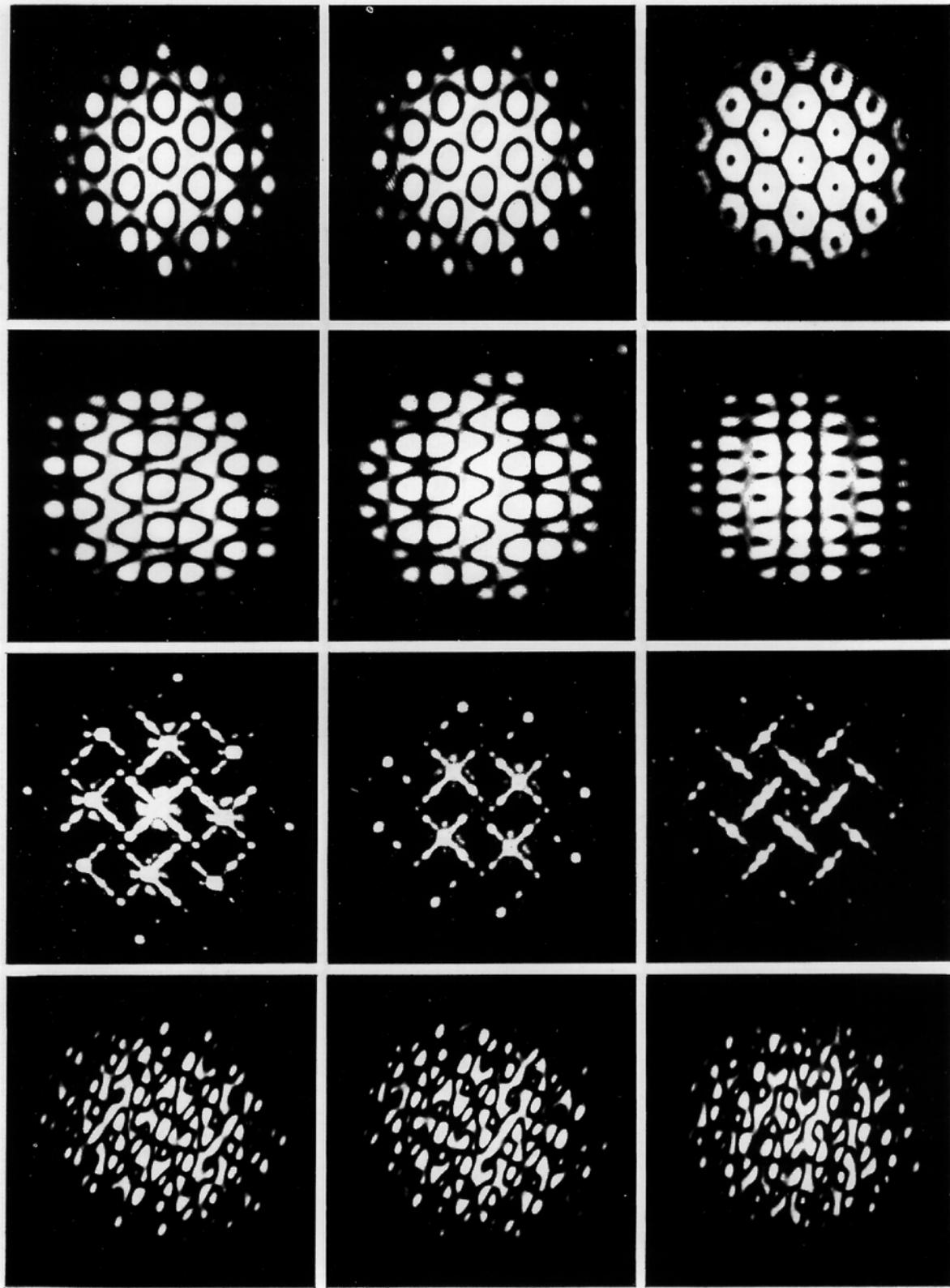


Plate 29

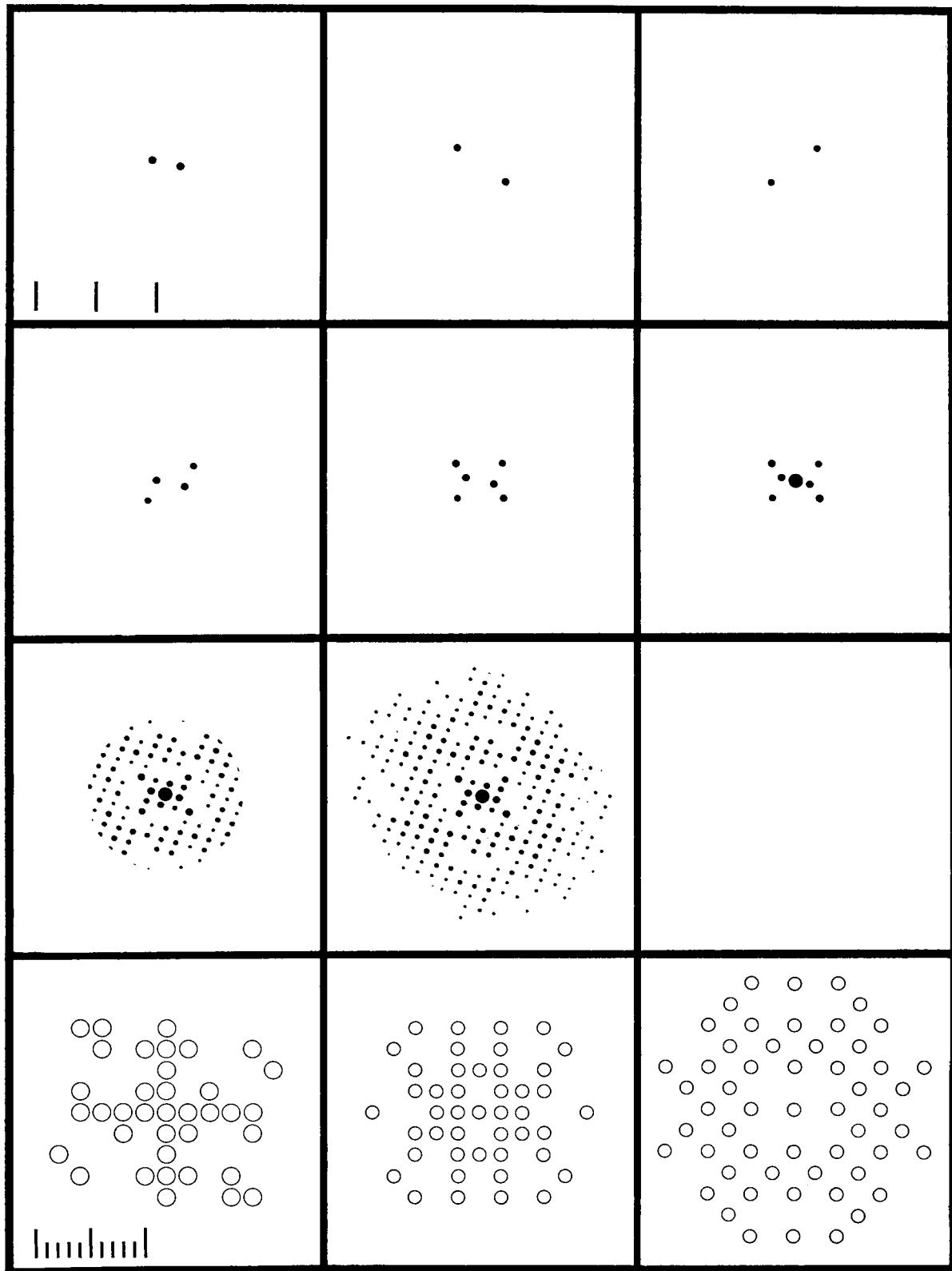


Plate 29

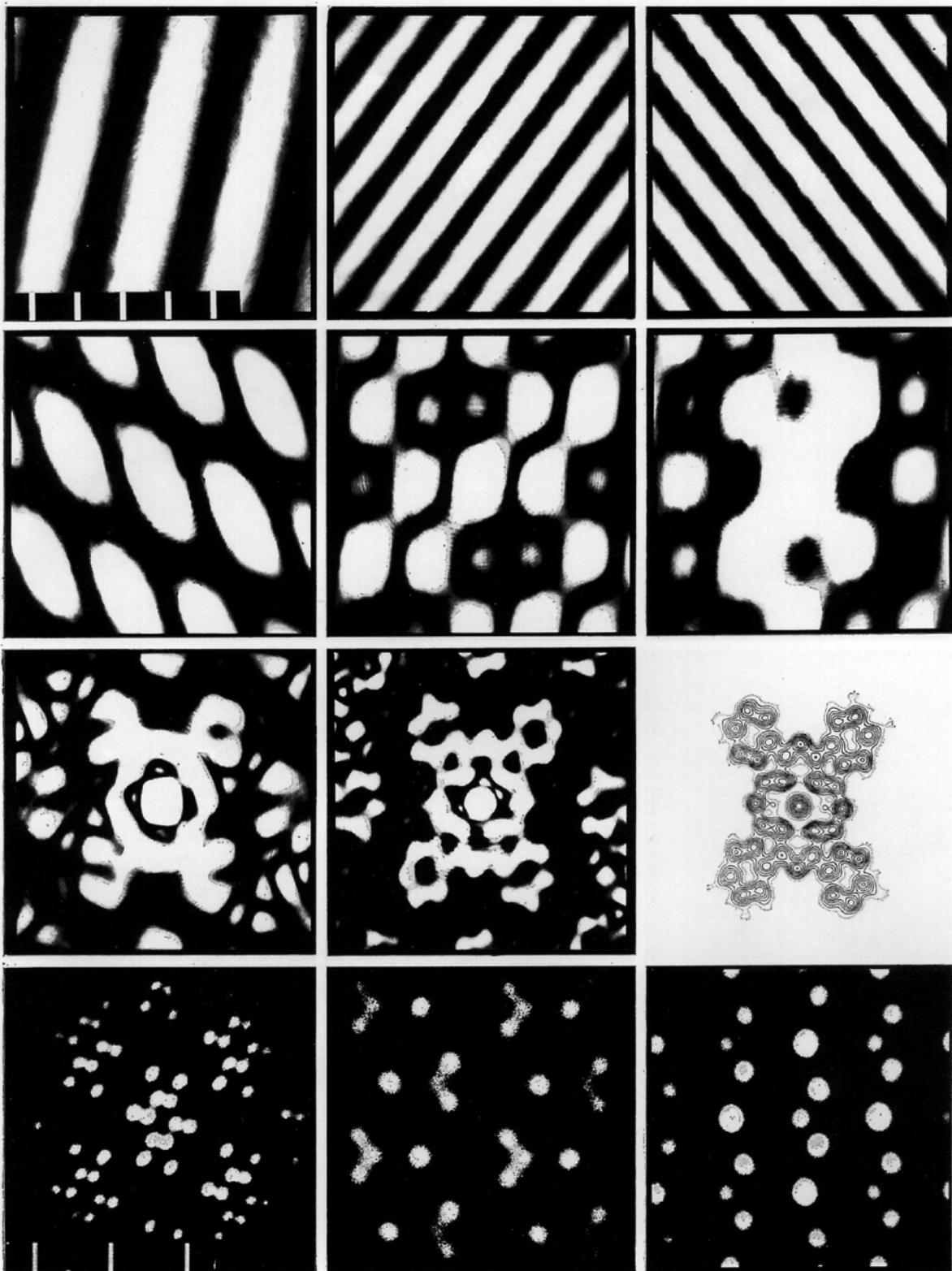


Plate 30

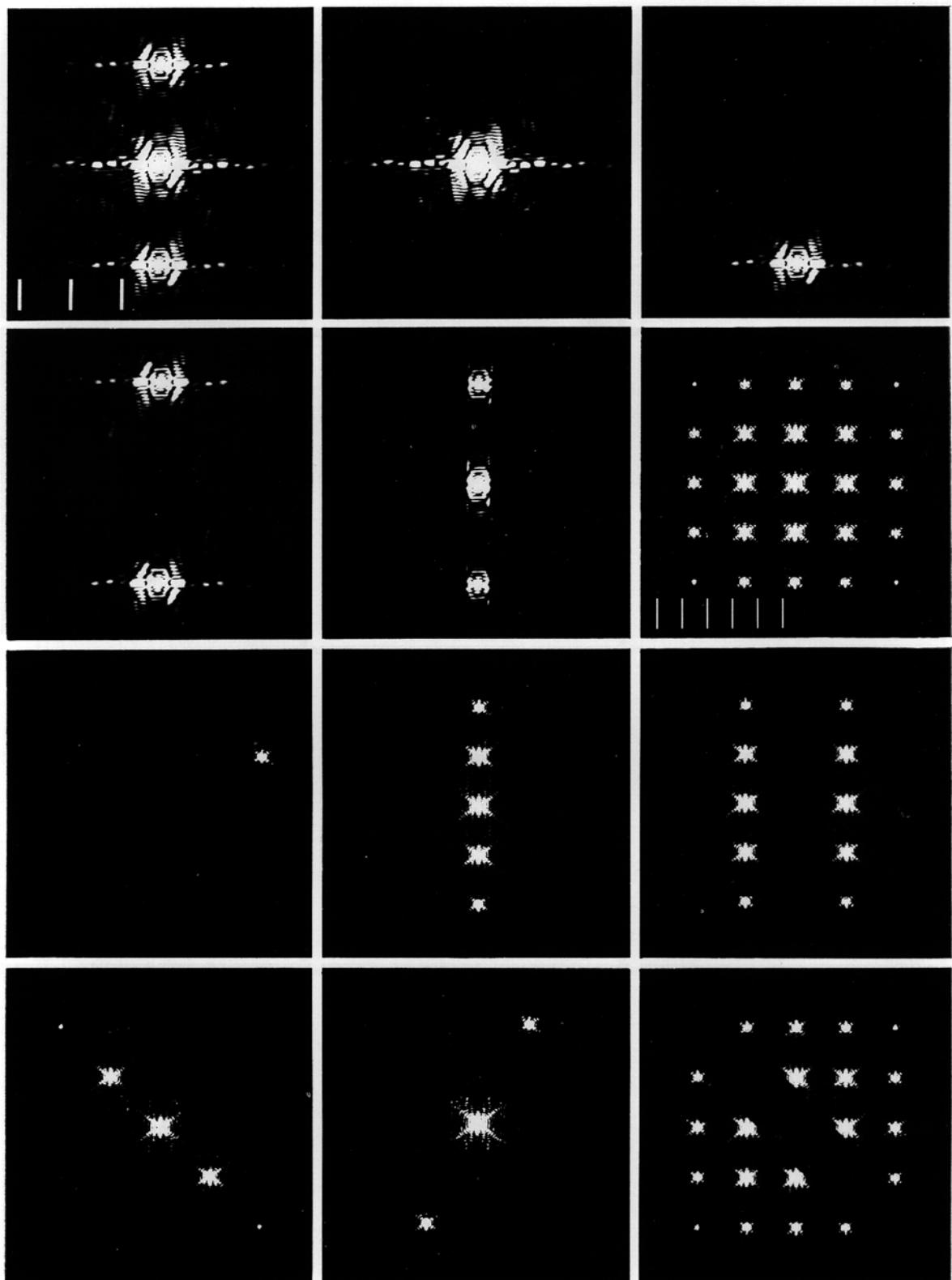


Plate 30

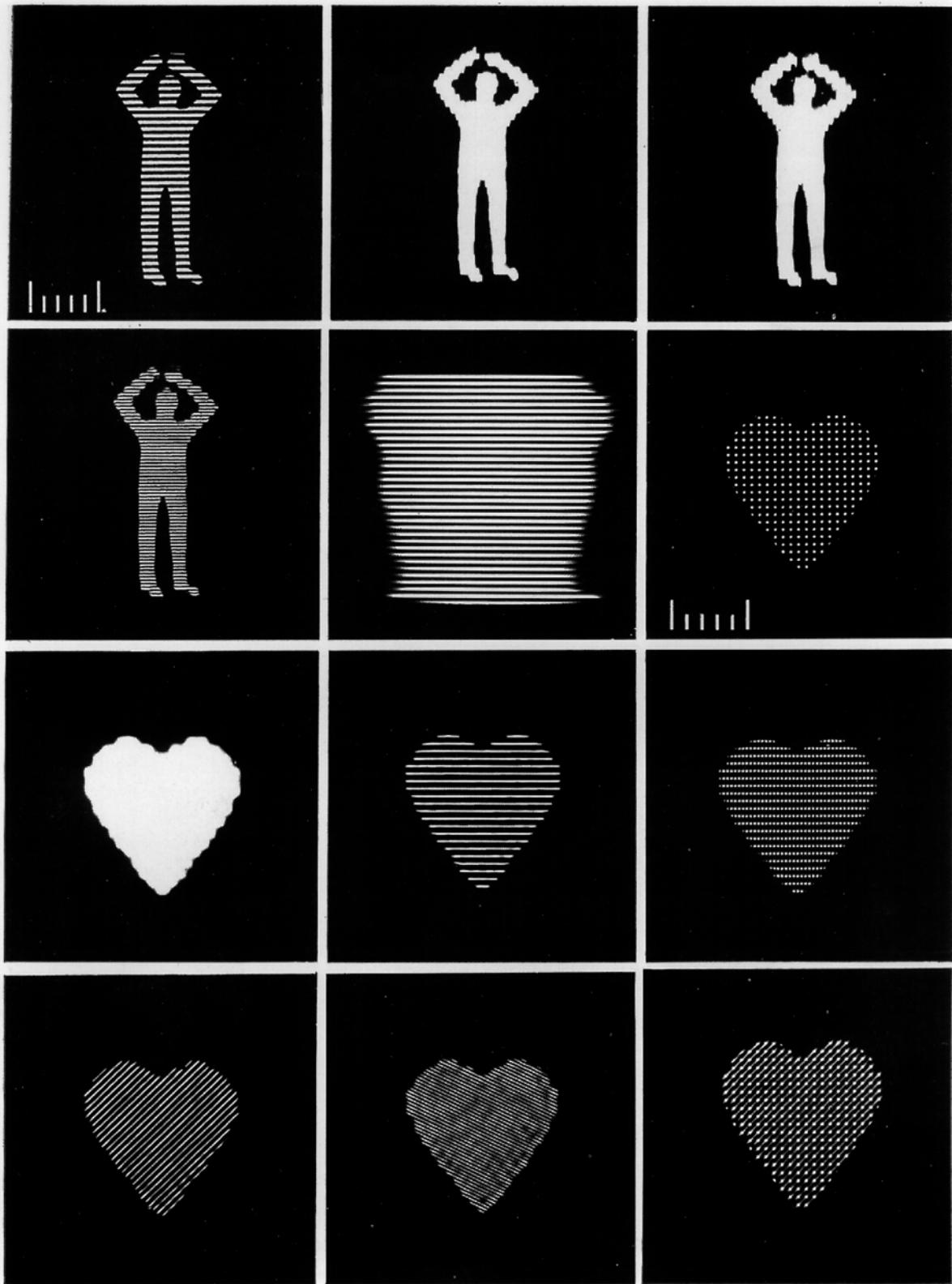
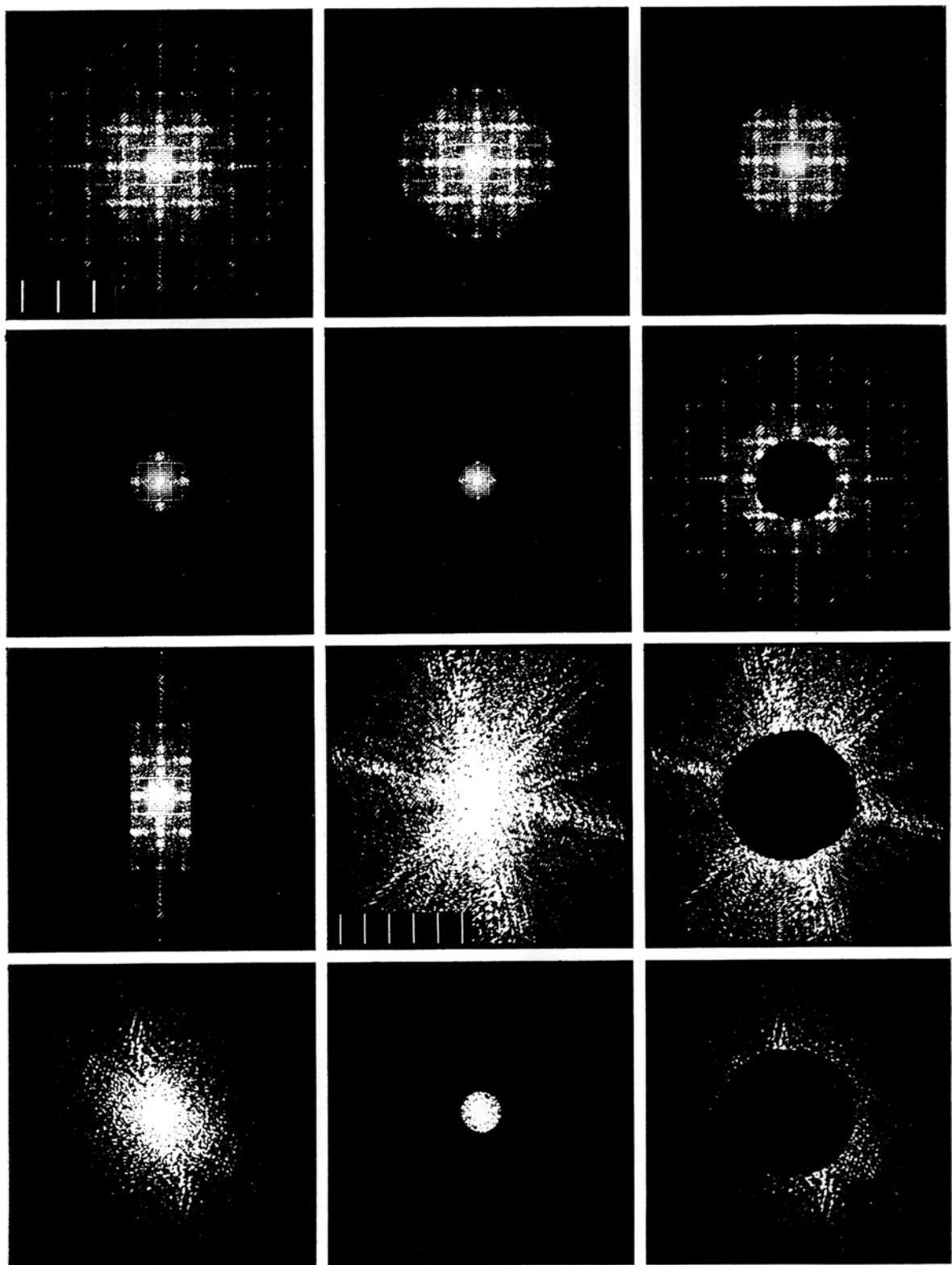


Plate 31



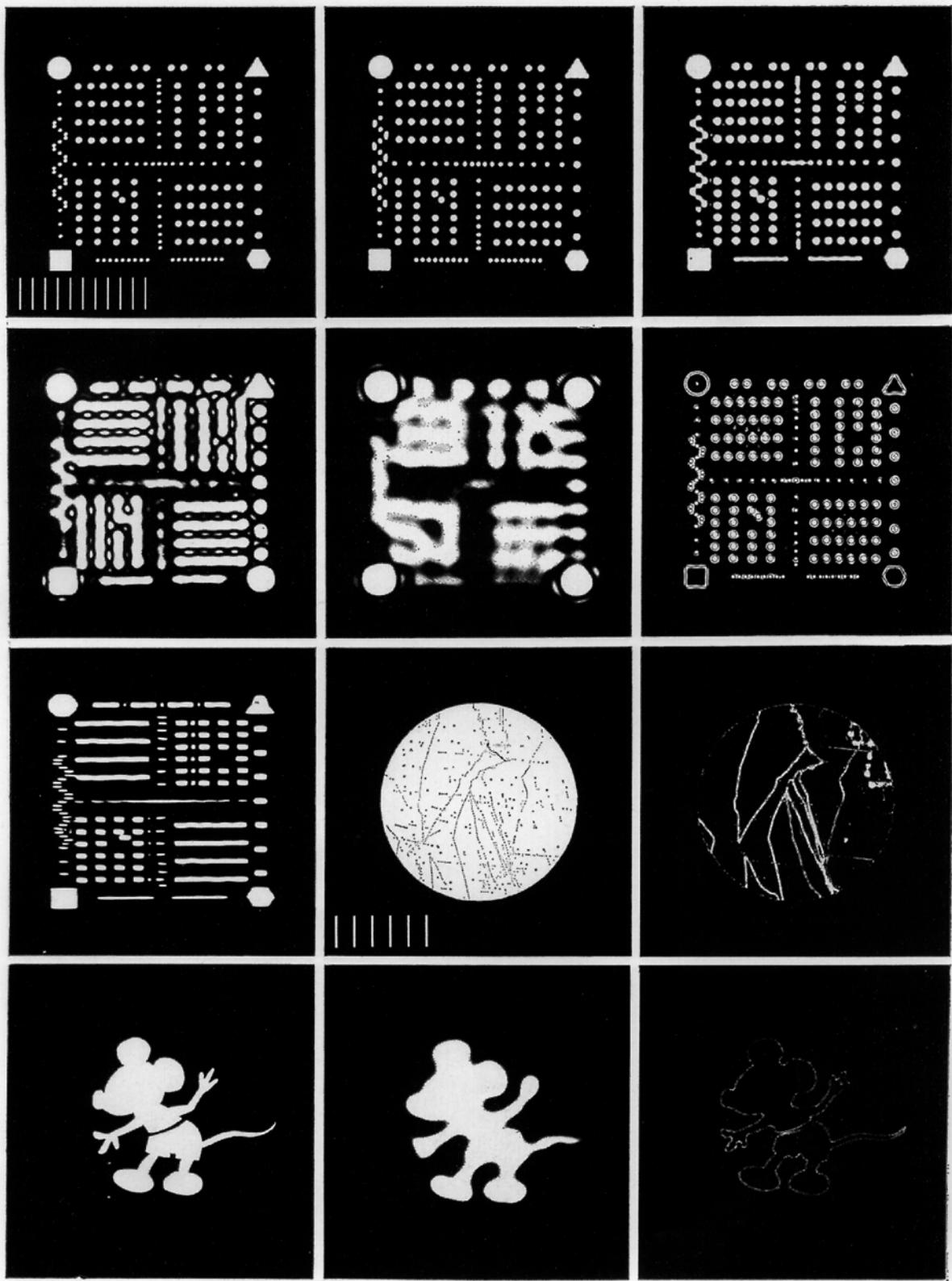
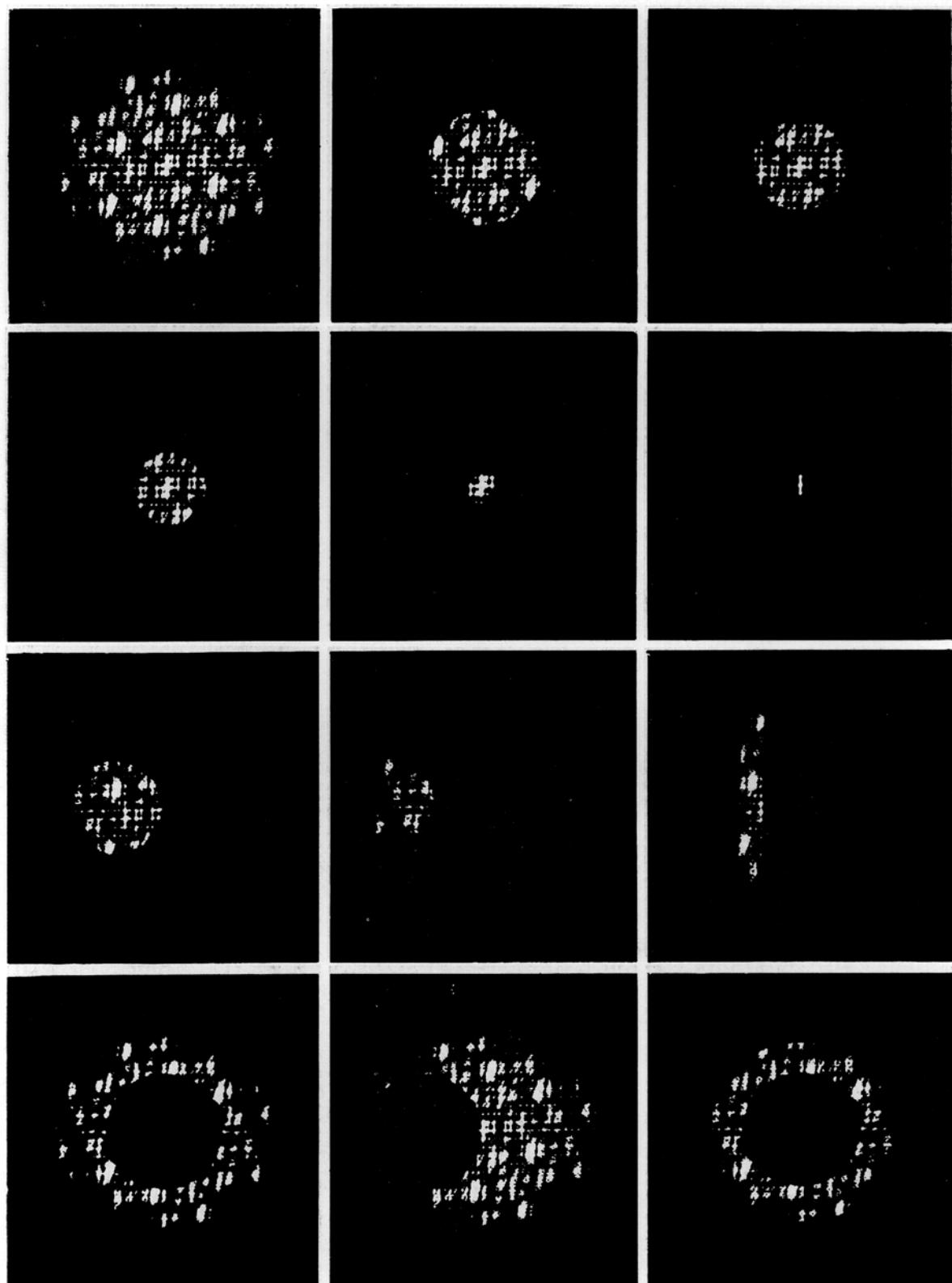
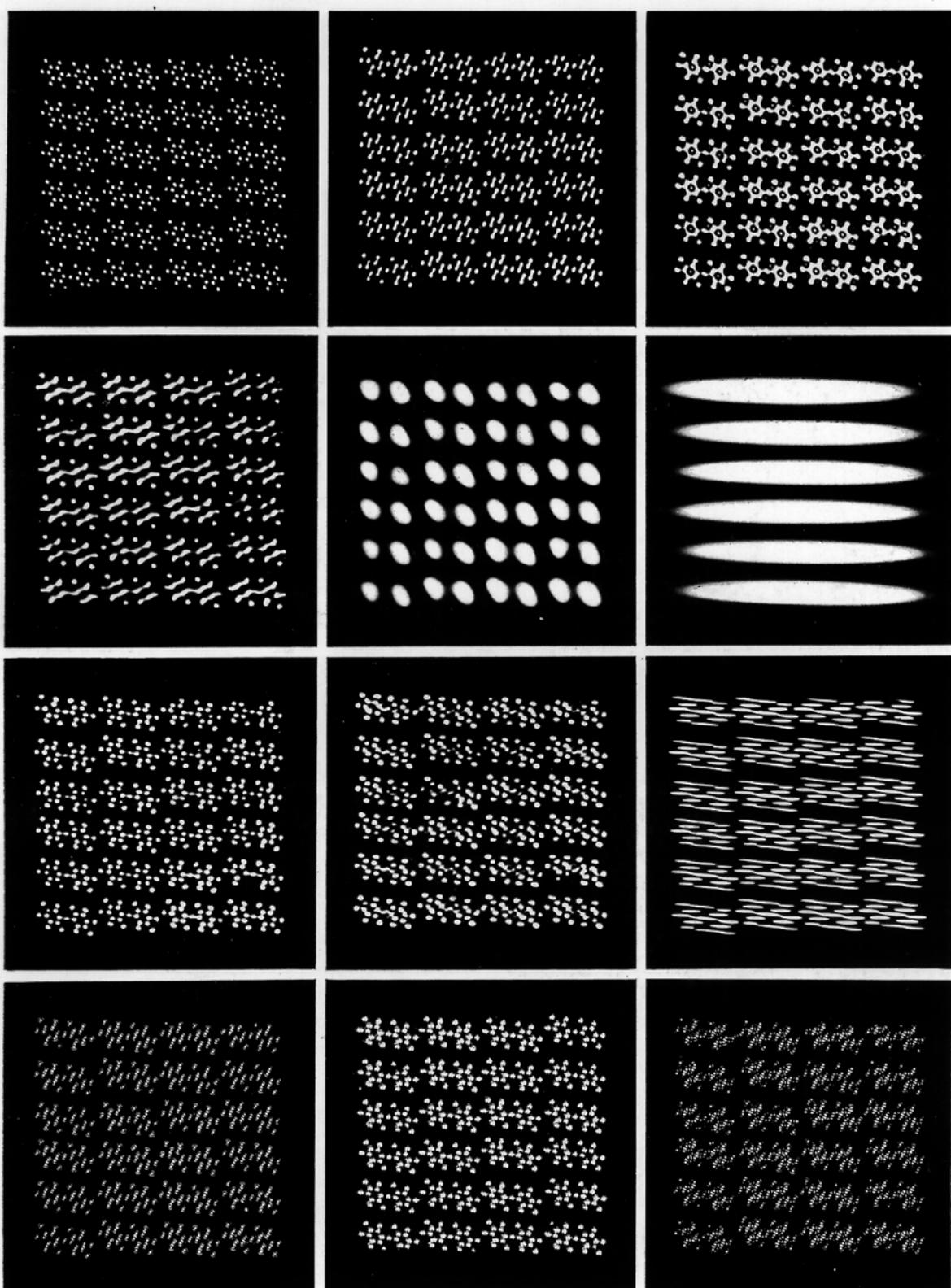


Plate 32



1 mm



1 mm

Appendix 2

Notes on the plates

Plate 1 Simple shapes and spacings

In each horizontal row the size and shape of the diffracting aperture is the same; in each vertical column the dispositions of the centres of the apertures are the same. The plate illustrates the idea of convolution in real space and multiplication in reciprocal space.

Plate 2 Superimposed fringes

The sequence shows how the diffraction pattern of a simple object is built up by superposition of sets of fringes.

Plate 3 Two hexagons

A continuation of Plate 2. The effect of adding further holes to make a hexagon of twice the scale of the first one is shown.

Plate 4 Combination of hexagonal arrangements

On this plate all the masks can be thought of as representations of idealised chemical molecules based on benzene.

Plate 5 Addition

Various aspects of the addition theorem in Fourier transformation are illustrated. In particular the addition of a diffracting unit at a centre of symmetry leads to enhancement of the positive (or in-phase) regions and diminution of the negative regions of the diffraction patterns, so providing a 'sign determination' procedure (2 and 3). Additions with respect to different origins are also illustrated.

Plate 6 The effect of orientation

The upper row shows three different planar molecular representations. In each successive row the diffracting masks are two-dimensional projections of the molecules in the upper row subjected to identical rotations in space.

Plate 7 Orientation

This plate is similar to Plate 6, but one object only is used and although the projections of the rotations have been done rather crudely and irregularly the patterns are still clearly interpretable.

Plate 8 Symmetry operations

In each of the vertical columns the basic object is the same. The object for the left-hand column has no symmetry, that for the centre column has a plane of symmetry, and that for the right-hand column has a two-fold axis perpendicular to the page. In the second horizontal row two objects are combined with a lateral translation, in the third row they are combined with a two-fold axis and in the fourth they are combined with a mirror plane.

Plate 9 The contribution of atoms in a unit cell to a particular X-ray reflection

1–3. The separations of the eleven principal spots on the centre vertical row of the diffraction patterns are reciprocally related to the spacing of the full lines in the masks. The distribution of the ‘atoms’ along the lines alters the rest of the pattern but these eleven spots remain strong.

4. The situation of some atoms in positions midway between the full lines affects the centre vertical row but alternate spots are still strong.

5. Vertical shifts do not affect the strong peaks, it is only the spacing of the rows that is important.

6. The atoms are no longer distributed along equally-spaced lines and the strong reflections are missing.

7–9. The atoms are again distributed along the lines but, in each case, the overall distribution is centrosymmetric, and consequently, the diffraction patterns have sharply defined zero lines. The corresponding Fourier transform is real.

10–12. Three different arrangements of atoms giving three different patterns. In each mask the atoms are at the intersections of three different sets of parallel lines—that is, at selected points of a lattice. In all the patterns the reciprocal lattice points are strong even though the rest of the pattern is different in the three cases.

Plate 10 Development of a lattice

A single aperture is repeated to build up rows and columns which are combined to produce the lattice of 12. Subsidiary diffraction maxima due to the small number of apertures can be seen clearly.

Plate 11 Lattices

The same basic unit of structure (which may be thought of as a chemical molecule) is used to build up twelve different crystal lattices. The overall multiplication by the transform of the basic unit is obvious in all twelve diffraction patterns.

Plate 12 Diffraction by a crystal

A crystal can be broken down into four component functions. The lattice, the scattering centre (atom), the scattering unit (molecule) and the bounding surfaces. These functions are shown in various combinations. The plate illustrates multiplication and convolution in both real and reciprocal space.

Plate 13 Convolution and multiplication

The basic diffracting unit consists of either a circle, a square or a rectangle in either of two different orientations. These basic units are repeated on square or rectangular lattices. Various shapes are used to limit the extent of the lattice that is included in each mask.

Plate 14 Circular and spiral lattices

A number of circular and spiral lattices, inspired by the structures of fibrous minerals such as chrysotile, are shown. See Whittaker (1955).

Plate 15 Perfect and paracrystalline lattices

1. Perfect square lattice.
2. Perfect rectangular lattice.
3. Perfect hexagonal lattice.
4. The same basic lattice as 1 but each point has been displaced horizontally from its original position by an arbitrary amount of up to 10% of the lattice spacing.
5. Paracrystal. Lattice points are confined to rows and columns but only the spacing of the horizontal rows is perfect. The horizontal spacing within each row is subject to a 10% variation and the register between a point in one row and the corresponding position in the next row is also subject to a 10% variation.
6. As 5 but with a larger (~25%) variation in the spacing and register.
7. Similar to 4 but the displacements are now two-dimensional.
8. Paracrystal. Lattice points are still confined to rows and columns but both the spacings within rows and columns and the register between corresponding points in adjacent rows and columns are subject to 10% variations about the mean value.
9. As 8 but with larger (~25%) variations in spacing and register.
10. Each horizontal row is a perfect one-dimensional lattice but the register of each row is subject to a 10% variation relative to the preceding row.
11. A paracrystal for which the unit cells are parallelograms of equal side but the cell angles vary.
12. As 11 but the magnitude of the cell side varies in addition to the variation in the cell angles.

The asymmetry of the diffuse intensity peaks in numbers 5, 6, 8 and 9 is a consequence of the method used for generating the arrays.

Plate 16 Gas and powder patterns

The diffracting screens represent projections of three-dimensional distributions of different atomic groups.

1. Single 'atoms' are positioned randomly; a monatomic gas.
2. Single 'benzene molecules' are positioned randomly but each has the same orientation with respect to axes in, and normal to, the plane of the paper.
3. The same as 2 but the benzene molecules are replaced by a small two-dimensional crystallite.
4. Pairs of atoms with bonds aligned are positioned randomly.
5. Benzene molecules positioned randomly, but having an arbitrary rotation about an axis in the plane of the paper.
6. Small crystallites positioned randomly but with arbitrary rotations about an axis normal to the page.
7. Pairs of atoms randomly positioned but with arbitrary rotations about an axis normal to the page.
8. Benzene molecules randomly positioned but with arbitrary rotations about an axis normal to the page.
9. The same as 6 but with orientations tending to be a preferred value.
10. Pairs of atoms randomly positioned and with arbitrary orientations in three dimensions.
11. Benzene molecules randomly positioned and with arbitrary orientations in three dimensions.
12. Three dimensional crystallites with arbitrary orientations in three dimensions. The crystallites are arranged on a coarse lattice for convenience only. (A powder pattern.)

Plate 17 General disorder

Various kinds of disorder are illustrated, all based on the same square lattice and two different types of scattering object (a square and a hexagon). Numbers 1-3 and 4-6 illustrate the similarities and differences between 'thermal' and 'substitutional' disorder. Numbers 2, 5 and 8 show how, for substitutional disorder, the diffuse scattering is proportional to the difference between the transforms of the two types of scatterer. Numbers 6 and 9 illustrate the difference between rigid-body motion (i.e. where the hexagons move as a whole) and independent motion of the 'atoms'. Numbers 7, 10, 11 and 12 are examples of the effect of omitting individual atoms from an otherwise perfect array of hexagons; in 7 20% of atoms have been omitted at random whereas in 10 one atom from each hexagon has been omitted. In 11 and 12 two and three atoms respectively have been omitted from each hexagon.

Plate 18 Short-range order

All the masks are based on a square lattice of unit cells each containing one hole. In each example approximately half of the lattice sites are occupied. In the four rows of diffracting screens the degree of order decreases from left to right. Each row is derived from a

different type of perfect superlattice and may be classified according to whether 'atoms' tend to segregate or alternate in the two axial directions. Numbers 1–3 have a tendency to sideways segregation but vertically neither segregation nor alternation is preferred. Numbers 4–6 tend to sideways alternation and vertically neither segregation nor alternation is preferred. Numbers 7–9 have sideways alternation and vertical alternation. Numbers 10–12 have sideways segregation but vertical alternation. The asymmetry of the diffuse intensity peaks in Numbers 7–12, and particularly noticeable in 7 and 10, is a consequence of the method used to generate the arrays. For further details see Welberry and Galbraith (1973).

Plate 19 Stacking faults

The diffracting screens represent layers of atoms stacked vertically. Three types of layer A, B and C, which differ only in their horizontal displacement, are present, the displacements are 0, $1/3$, $2/3$ of a lattice spacing respectively. Hexagonal packing is represented by a perfect layer sequence ABABA ... or BCBCB ... or ACACA ... while the sequences ABCABCABC ... and CBACBACBA ... are the left-hand and right-hand cubic forms. In the disordered sequences two probability parameters, α and β , were used to produce the layer sequences and these are defined in the following way.

- α is the probability that after layers AB the next is A.
- $1-\alpha$ is the probability that after layers AB the next is C.
- β is the probability that after layers BA the next is B.
- $1-\beta$ is the probability that after layers BA the next is C.
- 0 is the probability that after layers BA the next is A.

In the above definitions, A, B and C may be rotated cyclically. The actual values used to generate the examples shown were:

	α	β		α	β		α	β
1.	1·0	1·0	2.	0·9	0·9	3.	0·7	0·7
4.	0·003	0·003	5.	0·1	0·1	6.	0·3	0·3
7.	0·0	1·0	8.	0·1	1·0	9.	0·3	1·0
10.	0·5	0·5	11.	0·1	0·5	12.	0·3	0·5

Plate 20 Thermally disturbed lattices

This Plate illustrates the way in which thermal perturbations of a real crystal lattice give rise to diffuse scattering in the neighbourhood of diffraction maxima. All diffraction screens are based on the perfect lattice of 1, and have been produced by displacing individual lattice points by an amount proportional to the amplitude of one or more 'thermal' waves. These waves are

2. One longitudinal wave travelling up the page.
3. One transverse wave travelling up the page.

4. One transverse wave travelling in an arbitrary direction.
5. The same wave as 4 but with greater amplitude.
6. One transverse wave travelling in the same direction as 4 and 5 but with a shorter wavelength.
7. One longitudinal wave travelling in the same arbitrary direction as 4.
8. One wave travelling in the same direction as 4 and 7 but having some transverse and some longitudinal character.
9. Two waves travelling in different directions but having the same vibration direction.
10. Two waves travelling in the same two directions as 9 but each is a pure transverse wave.
11. Six waves of various wavelength, direction and vibration direction.
12. Twenty-four waves of various wavelength, direction and vibration direction.

Plate 21 Diffraction effects from fibres. I

- 1–3. Three single chains of different detailed structure. The layer lines are already present in the diffraction patterns although there is no crystalline structure unless the periodicity along the chain itself is regarded as one-dimensional crystallinity.
4. Two units as for 1.
5. Similar to 1. Two out of the three ‘atoms’ of the basic repeating group are randomly displaced.
6. Similar to 1. The basic repeating group of three atoms is fixed but the positions of the group along the chain are randomly displaced from the perfect positions of 1.
7. Four units as for 1.
8. A single chain as for 1 but with bends introduced in the plane of the photograph.
9. A single chain as in 1. The chain is bent as in 8 and also twisted about the chain axis.
10. A complete crystallite built up from the single chain of 1.
11. As 10 but with random displacements of complete chains in the vertical direction only. Note the horizontal row of sharp spots in the diffraction pattern.
12. As 10 but with random displacements of complete chains in the horizontal direction only. Note the vertical row of sharp spots in the pattern.

Plate 22 Diffraction effects from fibres. II

1. As Plate 21–10 but with random rotations about each individual chain axis. The pattern has far more sharp spots than Plate 21–12.
2. As Plate 21–10 but with random twists about each chain axis. The pattern has even more sharp spots than Plate 21–12 and 22–1.
3. As Plate 21–10 but with random rotations of the chains about axes perpendicular to the plane of the mask.
4. As 3 but with random twists about the chain axes as well.
5. As Plate 21–10 but with bending of the chains in the plane of the mask.

6. As 5 but with twists about the chain axes as well.
7. Projections of about 350 'crystallites' each consisting of about 150 to 200 'atoms' arranged randomly along parallel, equidistant rows. The crystallites are randomly oriented in the plane of projection.
8. As 7 but with a high degree of preferred orientation about the vertical direction.
9. Similar to 7. A projection of a collection of reasonably well oriented crystallites simulating a simple cellulose structure.
- 10-12. A series showing the patterns produced by randomly sited voids in fibres. The void widths have a Gaussian distribution as do their lengths L and their three dimensional orientations θ to the vertical direction. The width distribution is the same for all three, the parameters for the length and angular distributions are as follows.

10. $\sigma_L/L \approx 0$; $\sigma\theta \approx 0$
11. $\sigma_L/L = 1/6$; $\sigma\theta \approx 0$
12. $\sigma_L/L = 1/6$; $\sigma\theta \approx 2\frac{1}{2}^\circ$

Plate 23 Helices

Along each horizontal row a helix is shown first as a continuous curve and then sampled at equal intervals along the curve in two different ways. Numbers 1-3 and 4-6 show helices of different pitch viewed along a direction normal to their axes. Numbers 7-9 and 10-12 use the same helix as 4 but the viewing direction is at different angles to the axis of the helix.

Plate 24 Coiled coils and double helices

The effects of changing the amplitude of the secondary coil, the number of turns per turn, and the sampling of the basic curve are illustrated. In addition two double helices are shown which may be compared with the single helices of Plate 23. In 8 and 9 the two helices are 180° out of phase whereas in 11 and 12 they are out of phase by an arbitrary amount.

Plate 25 Small-angle scattering

This series demonstrates that, irrespective of the detailed distribution of the scattering points, the diffraction at small angles depends on the broadest features of the diffraction screen.

Plate 26 Diffraction effects of a gauze

1-10. The masks of this series consist of two circular apertures covered by square-mesh gauzes in the same orientation. For each mask the gauze over the right-hand aperture is shifted by a definite fraction of the gauze repeat distance, in both horizontal and vertical directions, relative to the gauze over the left-hand aperture. The diffraction patterns at the reciprocal lattice points show phase effects dependent on the shifts. The shifts are as follows, the horizontal fraction stated first:

ATLAS OF OPTICAL TRANSFORMS

- | | | |
|---|--|-------------------------------|
| 1. 0, 0 | 2. $\frac{1}{4}, \frac{1}{4}$ | 3. $1/3, 1/3$ |
| 4. 0, $\frac{1}{2}$ | 5. $\frac{1}{4}, 1/3$ | 6. $1/3, \frac{1}{2}$ |
| 7. 0, $1/3$ | 8. $\frac{1}{4}, \frac{1}{2}$ | 9. $\frac{1}{2}, \frac{1}{2}$ |
| 10. 0, $\frac{1}{2}$ | 11. Enlargement of central region of 10. | |
| 12. Enlargement of central region of 9. | | |

Plate 27 Phase control with mica

This plate illustrates phase control over the beams transmitted by the apertures in the mask using mica in the ways listed in Appendix 1B.

1–3. Method 4. Mica plates in unpolarised light. The arrows over the apertures indicate the fast directions in the mica plates.

4–6. Method 5. Half-wave plates of mica in plane-polarised light. The phases of the transmitted beams are shown inside the circles representing the apertures.

7–9. Method 6. Mica plates tilted in unpolarised light. In 7 the phases are all 0. In 8, ϕ is an arbitrary phase value between 0 and π .

10–12. Method 7. Half-wave mica plates oriented in circularly-polarised light. The arrows on the masks indicate that only part of the rows of holes are shown. To avoid interference effects between the two rows of holes separate exposures of their individual diffraction patterns were made on the same piece of film. The fringes from the smaller diameter holes are used as fixed marks against which the movement of the fringes from the larger set of holes can be judged. In 10 the phases of all the transmitted beams are the same; in 11 they increase by increments of $2\pi/3$ between adjacent apertures and in 12 the increment is π .

Plate 28 Non-central sections of three-dimensional transforms

A non-central section of the reciprocal solid can be recorded if it is moved to the centre by altering the phases of the light beams transmitted at the apertures, see Harburn and Taylor (1961). In all cases the phases have been altered by method 7 of Appendix 1B. The masks shown in the left-hand column transmit all beams with the same phase, in all other cases the phases are shown within the circles representing the apertures.

1–3. A tilted benzene ring.

4–6. A benzene ring in the boat and chair conformations.

7–10. Pentaerythritol. Sections $hk0$, $hk1$ and $hk4$ respectively. Data from Llewellyn, Cox and Goodwin (1937).

10–12. Tetraethyl diphosphine disulphide. Section $hk0$, a non-central section for a hypothetical planar molecule, and $hk3$ respectively. Data from Dutta and Woolfson (1961).

Plate 29 Optical Fourier synthesis

- 1–9. This series shows various contributions to the synthesis of rhodium phthalocyanine. Amplitude control is by method 1, Appendix 1B. No phase control is necessary because the scattering from the large rhodium atom at the origin dominates the diffraction pattern. Dunkerley and Lipson (1955).
10. Projection of hexamethylbenzene. Amplitude control by method 3, phase control by method 5. Hanson and Lipson (1952).
11. Urea. Amplitude control by method 2, phase control by method 6. Wyckoff and Corey (1934).
12. Non-centrosymmetric projection of sodium nitrite. Amplitude control by method 2, phase control by method 7. Carpenter (1952).
- The amplitude and phase information for numbers 10–12 can be found in the references given.

Plate 30 Spatial filtering

The left-hand page shows examples of diffraction patterns after modification by various obstructions. The right-hand page shows the images formed, in the manner described in Appendix 1A, from the information remaining in the diffraction patterns. Numbers 1 and 6 show the complete diffraction patterns and the corresponding 'perfect' images.

Plate 31 Spatial filtering

Numbers 1, 8 and 10 are complete diffraction patterns. Numbers 1–7 show the effect on resolution of excluding information from the final image for a test object. The amount of error in image 4 is particularly interesting. The diffracting object for 8 was a piece of mica with steps and scratches on the surface; 9 is an example of central dark-ground microscopy.

Plate 32 Spatial filtering

Number 1 shows the diffraction pattern and image of part of a perfect crystal structure. The rest of the series illustrates the effect on the image of excluding various Fourier components from a crystal structure calculation.

Appendix 3

Bibliography

REFERENCES

- Carpenter, G. B. (1952) *Acta Cryst.*, **5**, 132.
Dunkerley, B. D. and Lipson, H. (1955) *Nature*, **176**, 81.
Dutta, S. N. and Woolfson, M. M. (1961) *Acta Cryst.*, **14**, 178.
Hanson, A. W. and Lipson, H. (1952) *Acta Cryst.*, **5**, 362.
Harburn, G. (1973) Chapter 6. 'Optical Fourier Synthesis' in *Optical Transforms*, edited by Lipson, H. S. New York: Academic Press.
Harburn, G., Miller J. S. and Welberry, T. R. (1974) *J. Appl. Cryst.*, **7**, 36.
Harburn, G. and Ranniko, J. K. (1971) *J. Phys. E: Sci. Instrum.*, **4**, 394.
Harburn, G. and Ranniko, J. K. (1972) *J. Phys. E: Sci. Instrum.*, **5**, 757.
Harburn, G. and Taylor, C. A. (1961) *Proc. Roy. Soc., A*, **264**, 339.
Hill, A. E. and Rigby, P. A. (1969), *J. Phys. E: Sci. Instrum.*, **2**, 1084.
Llewellyn, F. J., Cox, E. G. and Goodwin, T. H. (1937) *J. Chem. Soc.*, 883.
Taylor, C. A. and Lipson, H. (1964) *Optical Transforms*. London: Bell.
Welberry, T. R. and Galbraith, R. (1973) *J. Appl. Cryst.*, **6**, 87.
Whittaker, E. J. W. (1955) *Acta Cryst.*, **8**, 265.
Wyckoff, R. W. G. and Corey, R. B. (1934) *Z. Krist.*, **89**, 462.

ADDITIONAL BIBLIOGRAPHY

A short selection of papers and texts containing relevant material.

- Amoros, J. L. and Amoros, M. (1968) *Molecular Crystals: their Transforms and Diffuse Scattering*. Wiley: New York.
Beeston, B. E. D., Horne, R. W. and Markham, R. (1972) Chapter: 'Electron diffraction and optical diffraction techniques', from *Practical Methods in Electron Microscopy*. Edited by Glauert, A. M. North Holland: Amsterdam.
Bragg, W. L. (1939) *Nature*, **143**, 678.
Hosemann, R. and Bagchi, S. N. (1962) *Direct Analysis of Diffraction by Matter*. North Holland: Amsterdam.
Lipson, H. S. (1973) *Optical Transforms*. Academic Press: New York.
Lipson, H. and Taylor, C. A. (1958) *Fourier Transforms and X-ray Diffraction*. Bell: London.

APPENDIX 3 BIBLIOGRAPHY

33

- Parrent, G. B. and Thompson, B. J. (1969) *Physical Optics Notebook*. Society of Photo-optical instrumentation Engineers: California.
- Taylor, C. A. (1969) *Pure Appl. Chem.*, **18**, 533.
- Taylor, C. A. and Lipson, H. (1964) *Optical Transforms*. Bell: London.
- Taylor, C. A. and Ranniko, J. K. (1974) *J. Micros.*