Homework #6

2D Lattices, 2D Space Groups, and Inversion

Due 5pm Friday Nov. 22

Turn in outside of Durand 110 or email to duerloo *at* stanford.edu

1. Rotational Symmetries Commensurate with a Lattice (i.e. Translational Symmetry)

Consider two lattice points A and A' in a crystal connected with lattice vector $\vec{a}$. Draw a figure showing how these two points move when a rotation through angle α is applied at lattice point A. Since every operation in a group has an inverse operation, the rotation through $-\alpha$ should also be a member of the space group. Include on your figure the points generated when a rotation of $-\alpha$ is applied at lattice point A'. By considering that all points in a lattice must be related by a sum of integer multiples of lattice vectors, determine the values of alpha that are commensurate with a lattice. Write the conventional symbol for each of these rotations.

2. Identification of 2D Space Groups

Identify the primitive cell lattice vectors and all the symmetry elements that are present for the following structures. Take them to be 2D structures. Give the international ID symbols for the space and point groups. Are you sure that you've found all the symmetry elements rather than a subgroup of the full symmetry group? How can you be sure?

a) Graphene.
b) 2D BN. (2D BN atomic positions are identical to graphene, with B &N the two atoms in the unit cell.)
c) Pick one of the M. C. Escher drawings below.
d) Monolayer TaS_2 in the 1T phase (i.e. a monolayer unit from the CdI_2 phase). Recall that this monolayer is not atomically thin. Therefore we will consider only the 2D projection of the monolayer onto the (001) plane. Consider this monolayer to be one of the monolayers the CdI_2 structure crystal, $(\alpha B \gamma)$ stacking sequence, and draw a projection on the (001) plane.

A crystallographic description of the Escher figures is provided in "Fantasy and Symmetry: The Periodic Drawings of M. C. Escher" by Caroline H. MacGillavry, International Union of Crystallography 1975.

3. Centrosymmetry

Determine whether the point or space group for the following materials contains a center of symmetry and if so, determine its location. Note that it does not need to be located on an atom site. We will later see in class how materials without an inversion center have potential to be piezoelectric or to be used as a frequency doubling crystal (producing light of frequency 2ω from when light of frequency ω is shined into the crystal).

a) Diamond Silicon
b) Wurtzite ZnO
c) Sphalerite GaAs
d) CsCl
e) Graphene
f) Graphite
g) CaF_2
h) CdI_2
i) Monolayer BN

j) Silicon (111) crystal surface

Plate 16

Plate 24

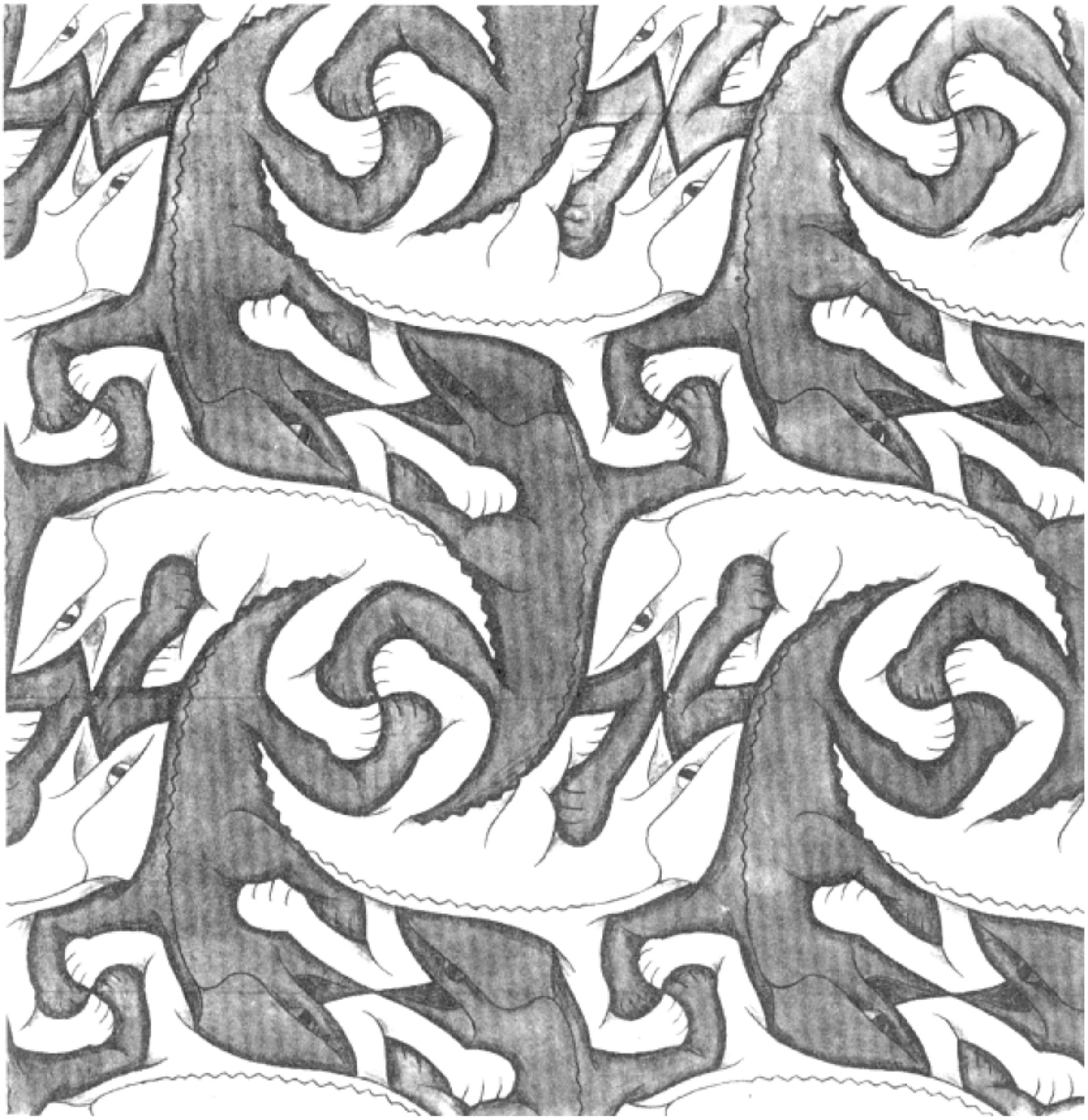

Plate 4

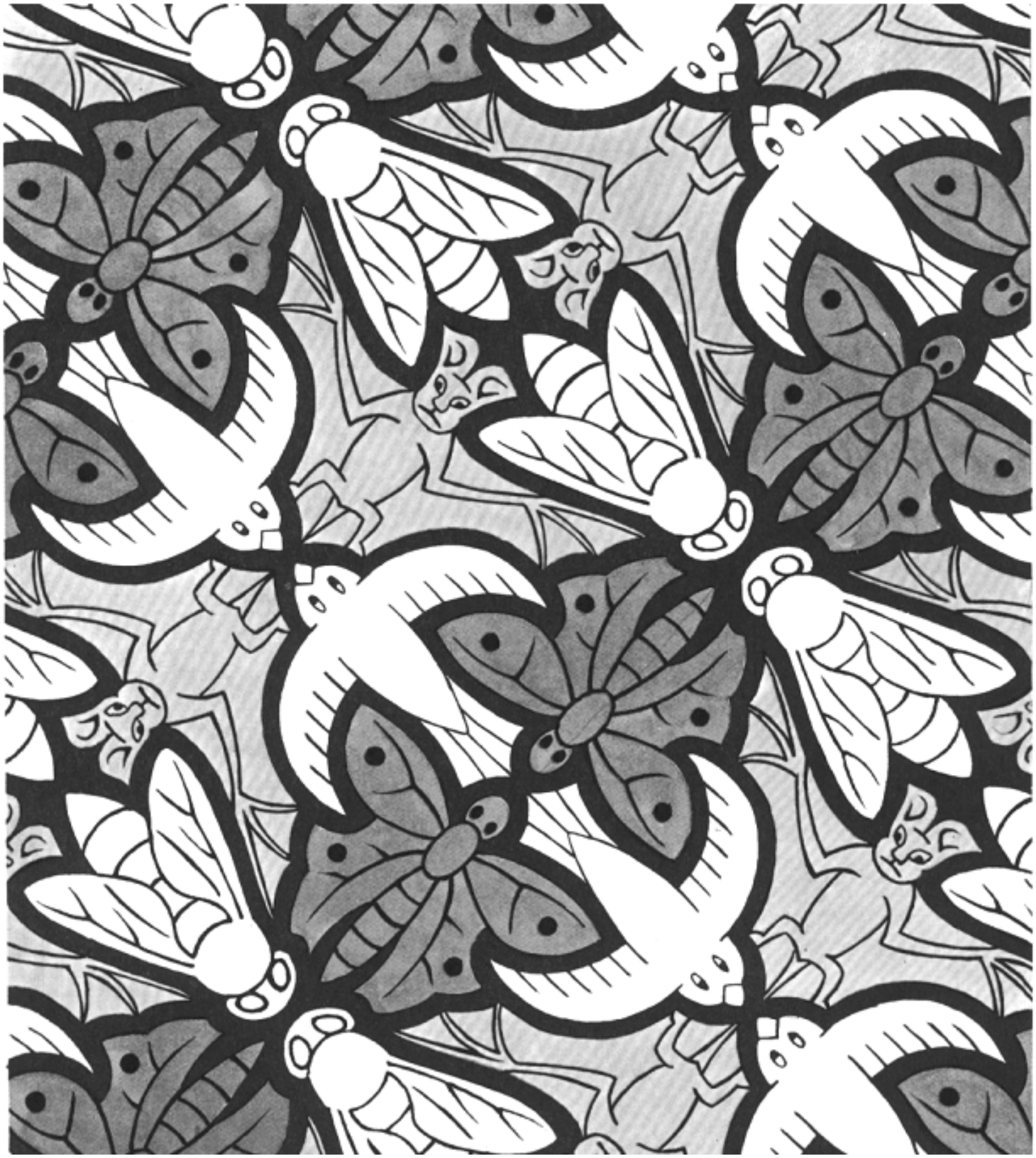

Plate 6

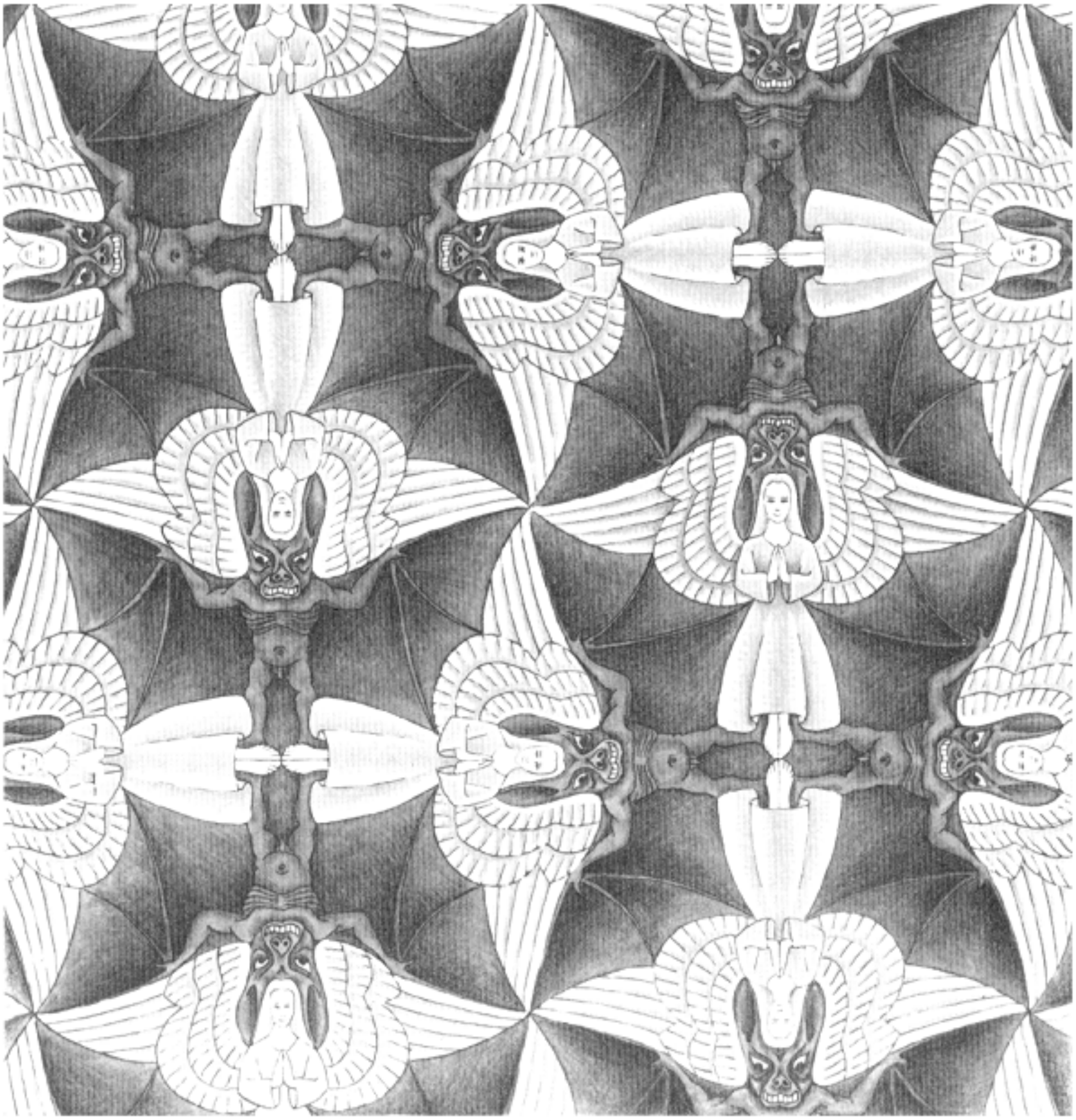

Plate 9

Plate 7 (Note: Ignore the shading change in this image.)

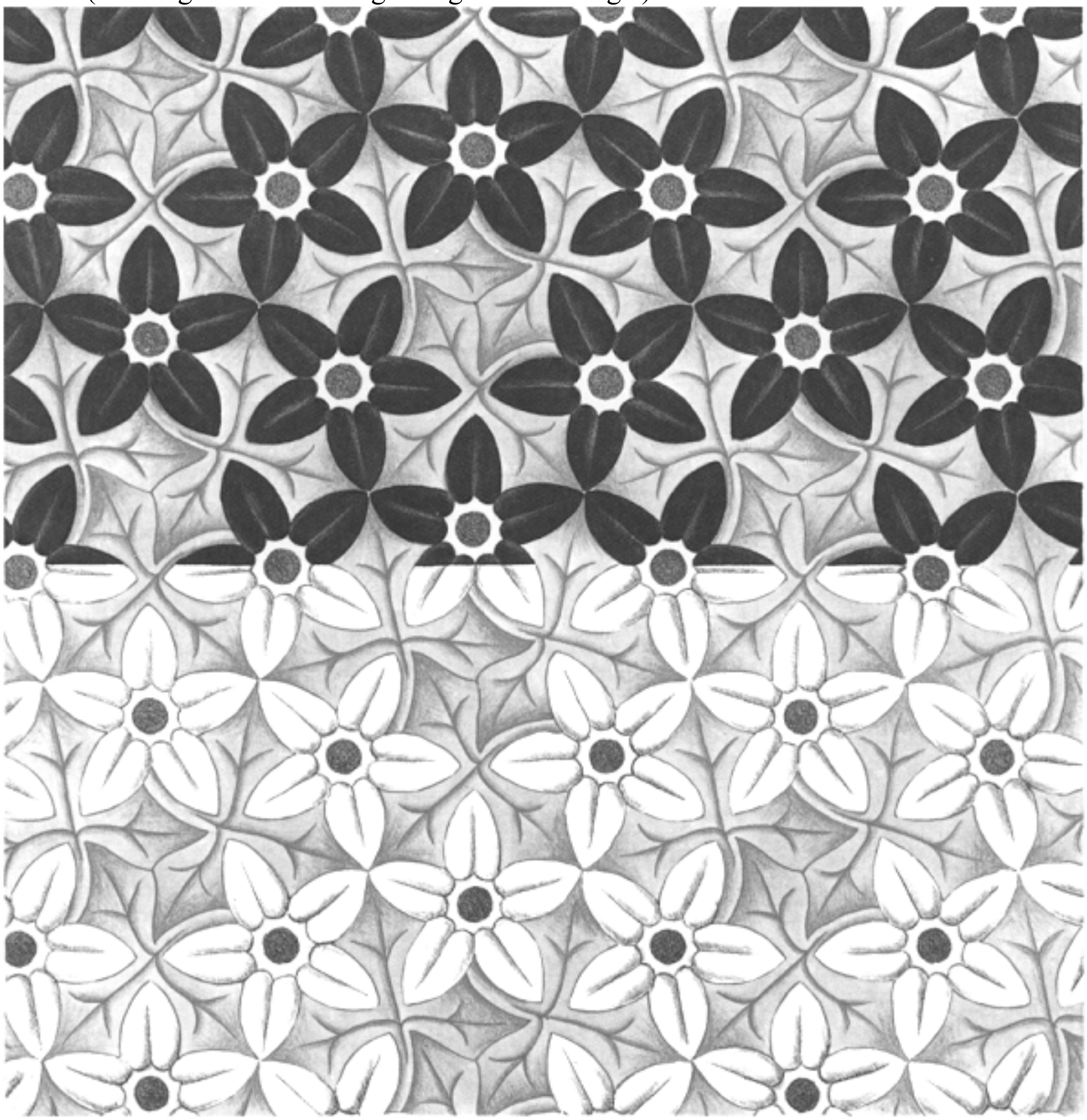

Plate 12

Plate 13

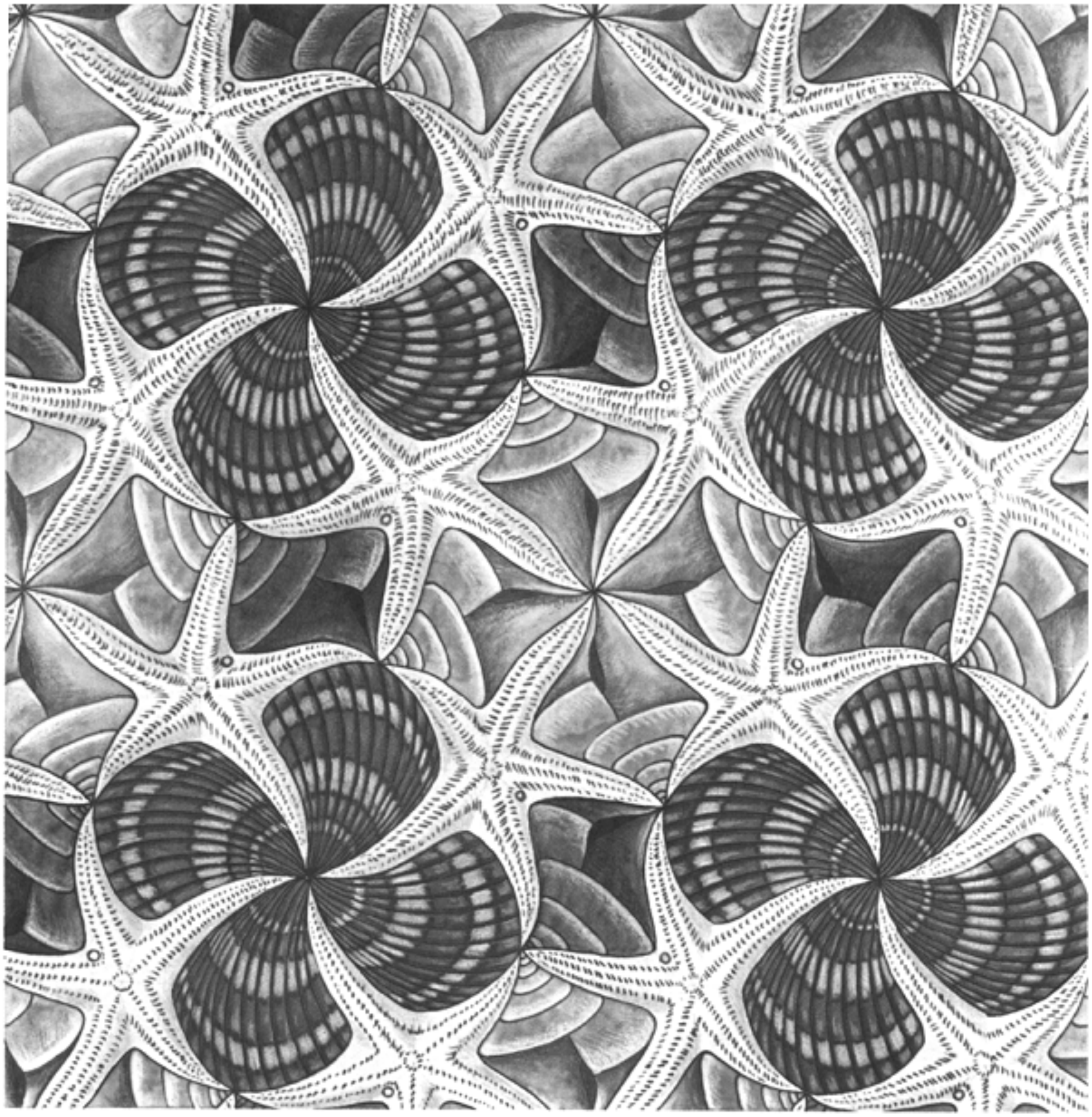

Plate 41