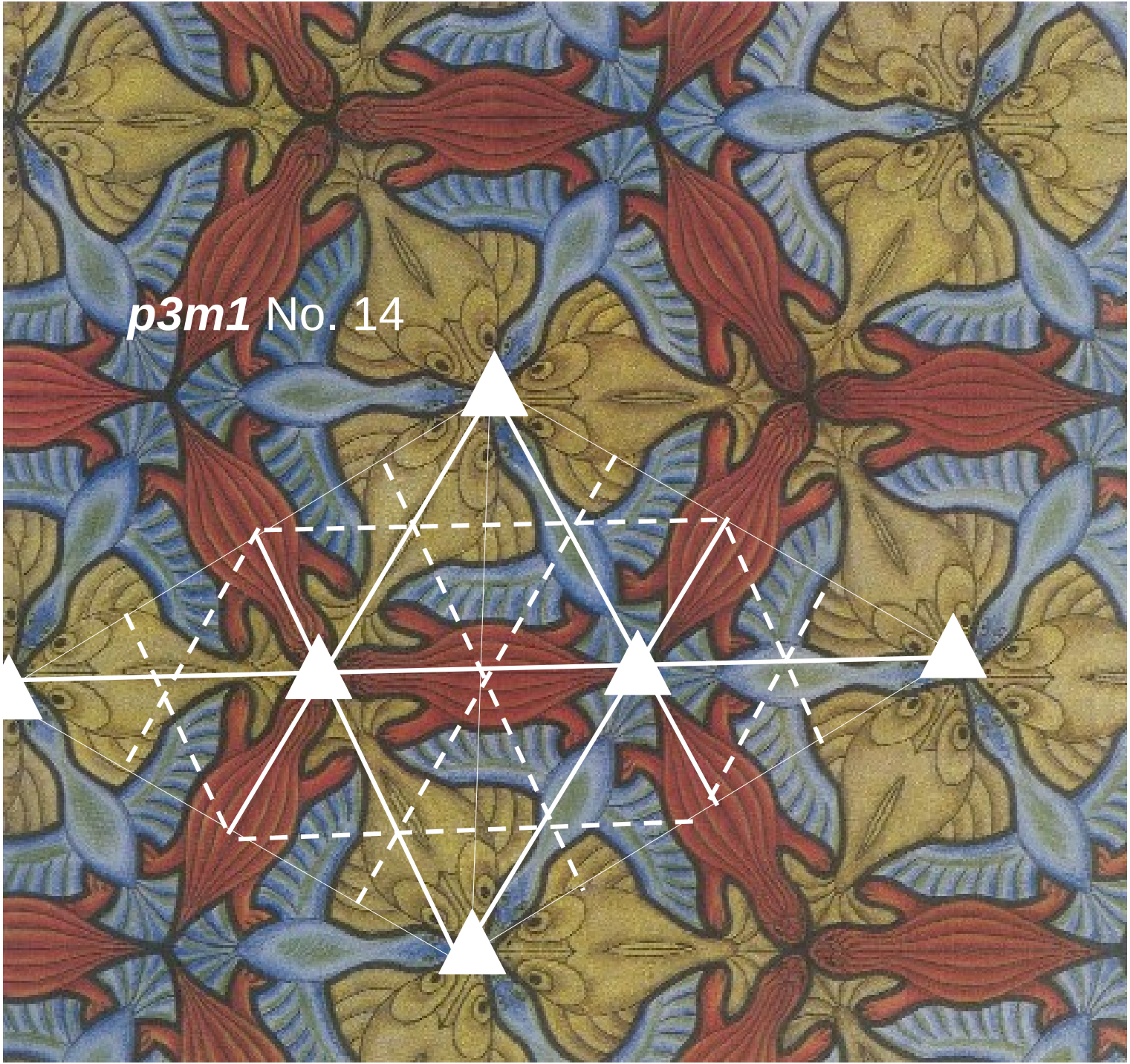
Symmetry, etc. Tutorial

P.G. Radaelli
ISIS Facility - RAL

ftp://ftp.nd.rl.ac.uk/scratch/UCL_Teaching_2007/

A phase transition in 2D

1. Examine the symmetry of the Escher drawing, and compare it with the IT entry.
2. Identify special positions and symmetry elements
3. Look at the modified drawing, with the colour pattern altered. Identify the lost symmetry elements.
4. Can you determine the low-symmetry space group?


p3m1 No. 14

Hexagonal

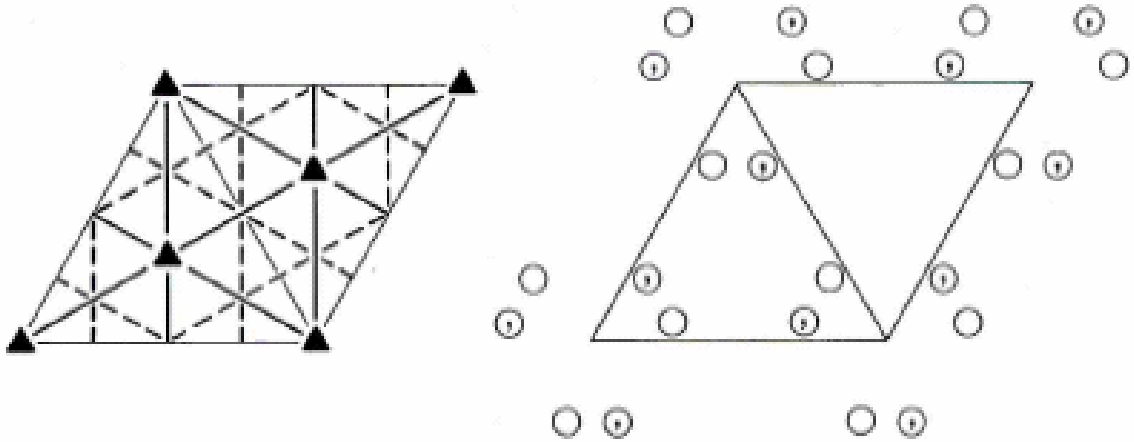
$3m$

$p3m1$

Patterson symmetry $p6mm$

$p3m1$

No. 14



Origin at $3m1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$

Symmetry operations

(1) 1	(2) 3^+ 0,0	(3) 3^- 0,0
(4) m $x,\bar{x}$	(5) m $x,2x$	(6) m $2x,x$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
6	*e*	1	(1) x,y (4) $\bar{y},\bar{x}$	(2) $\bar{y},x-y$ (5) $\bar{x}+y,\bar{y}$	(3) $\bar{x}+y,\bar{x}$ (6) $x,x-y$	General: no conditions
3	*d*	.*m*.	$x,\bar{x}$	$x,2x$	$2\bar{x},\bar{x}$	Special: no extra conditions
1	*c*	3*m*.	$\frac{1}{3},\frac{2}{3}$			
1	*b*	3*m*.	$\frac{2}{3},\frac{1}{3}$			
1	*a*	3*m*.	0,0			

Maximal non-isomorphic subgroups

I [2] $p3\,1\,1$ ($p3$, 13) 1; 2; 3
[3] $p\,1\,m\,1$ (cm, 5) 1; 4
[3] $p\,1\,m\,1$ (cm, 5) 1; 5
[3] $p\,1\,m\,1$ (cm, 5) 1; 6

IIa none

IIb [3] $h\,3\,m\,1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($p3\,1\,m$, 15)

Maximal isomorphic subgroups of lowest index

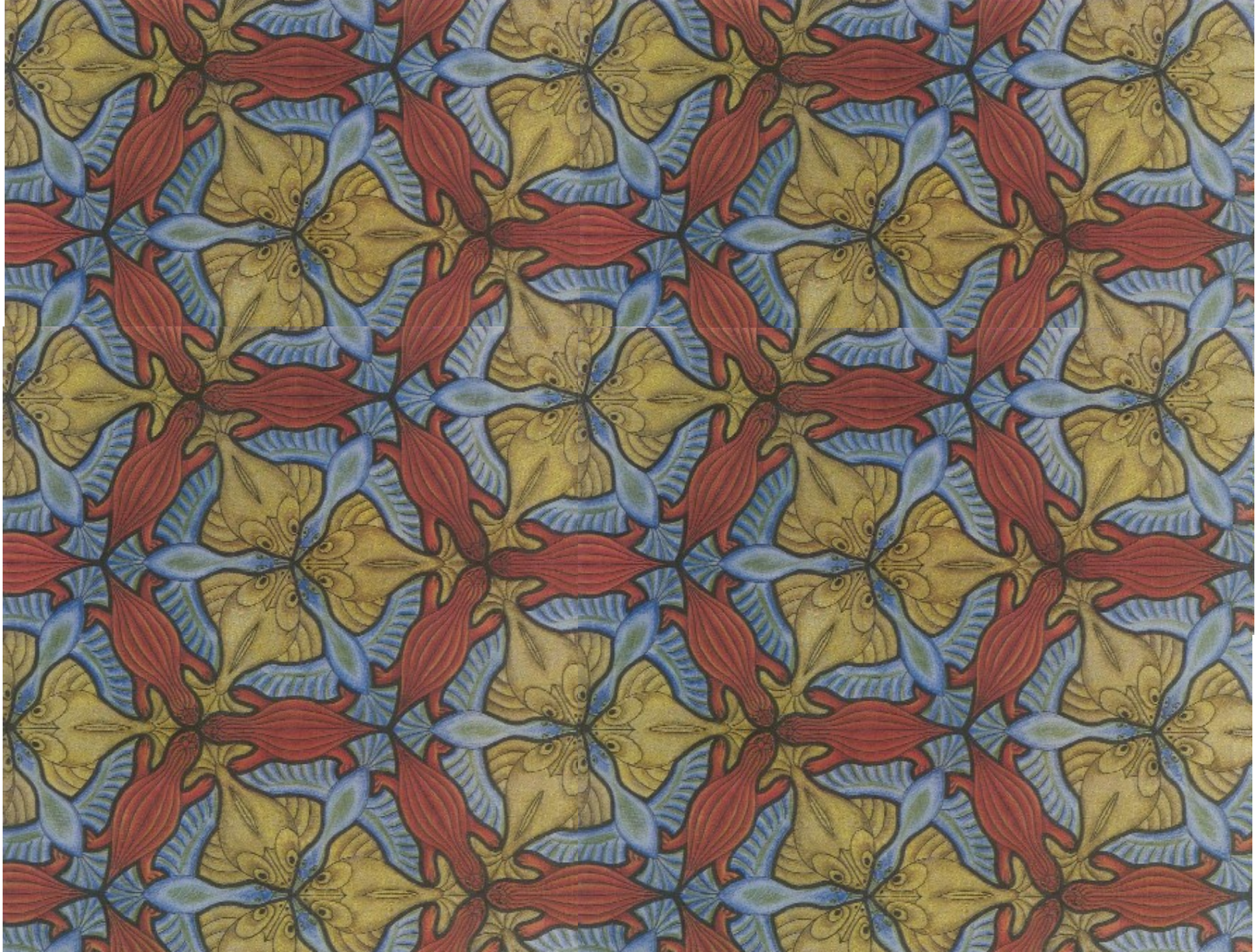
IIc [4] $p\,3\,m\,1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (14)

Minimal non-isomorphic supergroups

I [2] $p\,6\,m\,m$ (17)

II [3] $h\,3\,m\,1$ ($p3\,1\,m$, 15)

p3m1 No. 14




p3m1 No. 14