Examples Class 2: Stereographic Projections

Calcium Chloride

The orthorhombic unit cell of $CaCl_2$ has $a = 0.624\,\text{nm}$, $b = 0.643\,\text{nm}$ and $c = 0.420\,\text{nm}$ with ion positions at

Ca: 0,0,0 $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

Cl: $x, y, 0$ $\overline{x}, \overline{y}, 0$ $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2}$ $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2}$

with $x = 0.325$ and y= 0.275. Fig. 1 is an accurate projection of this structure on (001).

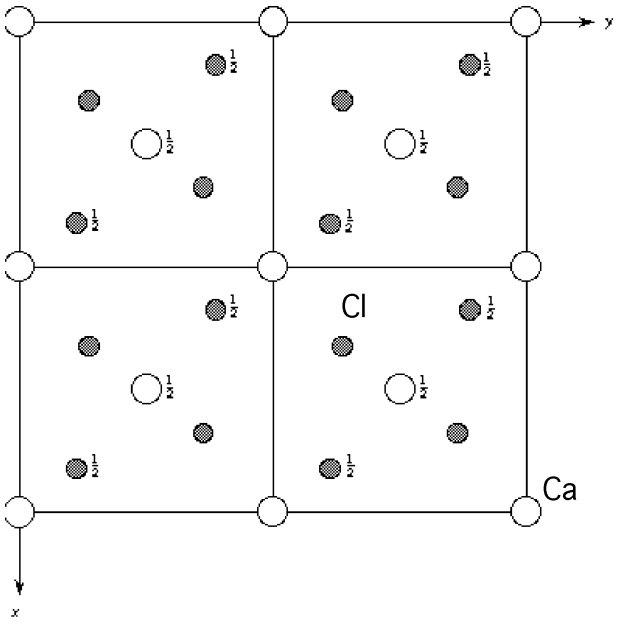

Figure 1: The structure projection for calcium chloride

1. What is the Bravais lattice of this structure?
2. Locate all symmetry elements present in the structure and hence determine those along [100], [010] and [001]. What is the point group of the crystal structure?
3. Determine the point symmetries of the Ca and Cl ions and express them on sketch stereograms.

Calcite

Calcite is trigonal with $c/a = 0.854$ and $\{10\bar{1}1\}$ cleavages. It belongs to the crystal class $\bar{3}m$.

1. Show that $(0001) : (10\bar{1}1) = 44.6°$ and $(0001) : (01\bar{1}2) = 26.2°$.
2. Draw an accurate 127 mm diameter stereogram centred on 0001, as illustrated in Fig. 2. Show on it the poles of the $\{10\bar{1}1\}$ cleavage planes and their corresponding traces. Add the pole of a section parallel to $(01\bar{1}2)$ along with its trace.
3. From an inspection of your stereogram, draw a sketch of the permitted vibration directions relative to the cleavage traces when light is incident normally on the $(01\bar{1}2)$ section of a thin crystal of calcite.

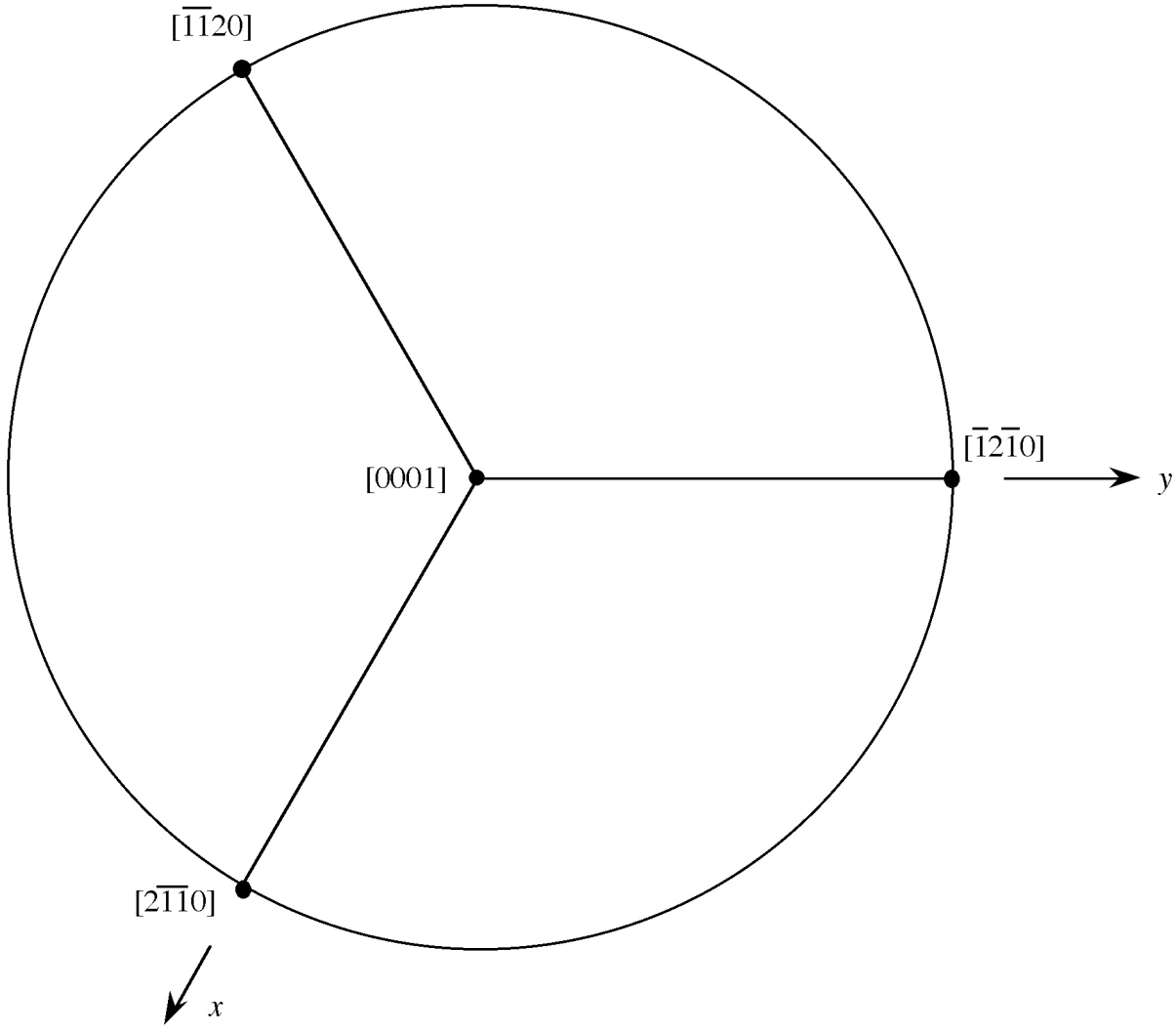

Figure 2: Stereogram

Coincidence Site Lattice

Fig. 3 is a template of a primitive cubic lattice (basis symbol 'X') projected onto (001). Fig.4 on the transparency is identical (basis symbol 'Y') but with the dots replaced by crosses. You are provided with a transparency pen.

By rotating the transparency with respect to the template, determine the Σ value of the coincidence site lattice produced by a rotation of 36.9° about [001]. What are the basis vectors of the CSL in terms of the primitive cubic lattice?

The rotation matrix relating the two primitive cubic lattices for a right–handed rotation θ about a unit axis $[u_1\ u_2\ u_3]$ is given by:

$$(\mathrm{Y\ J\ X}) = \begin{pmatrix} u_1u_1(1-m)+m & u_1u_2(1-m)+u_3n & u_1u_3(1-m)-u_2n \\ u_1u_2(1-m)-u_3n & u_2u_2(1-m)+m & u_2u_3(1-m)+u_1n \\ u_1u_3(1-m)+u_2n & u_2u_3(1-m)-u_1n & u_3u_3(1-m)+m \end{pmatrix} \tag{1}$$

where $m = \cos\theta$ and $n = \sin\theta$

Verify the Σ value obtained graphically using this matrix.

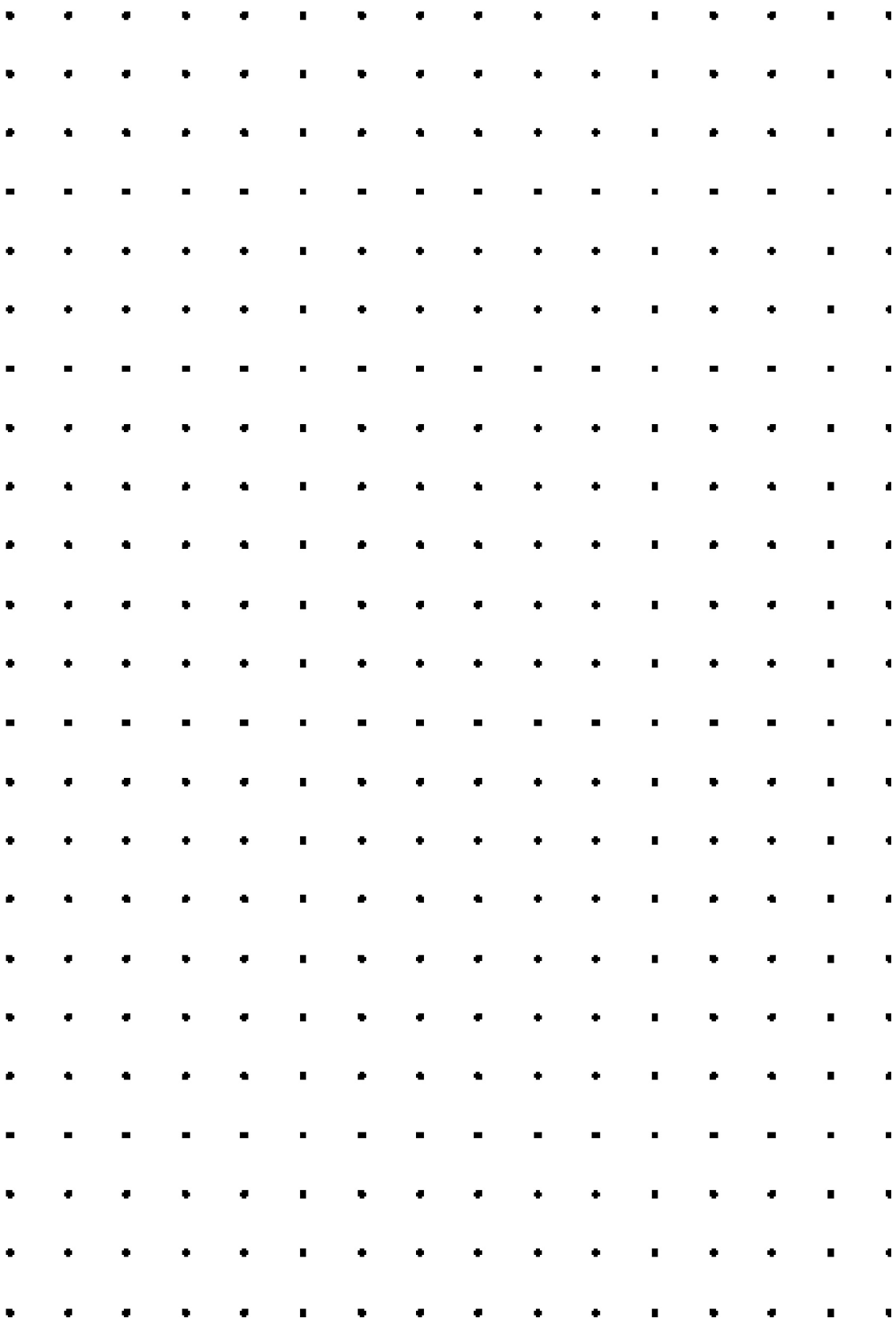

Figure 3: Template 1

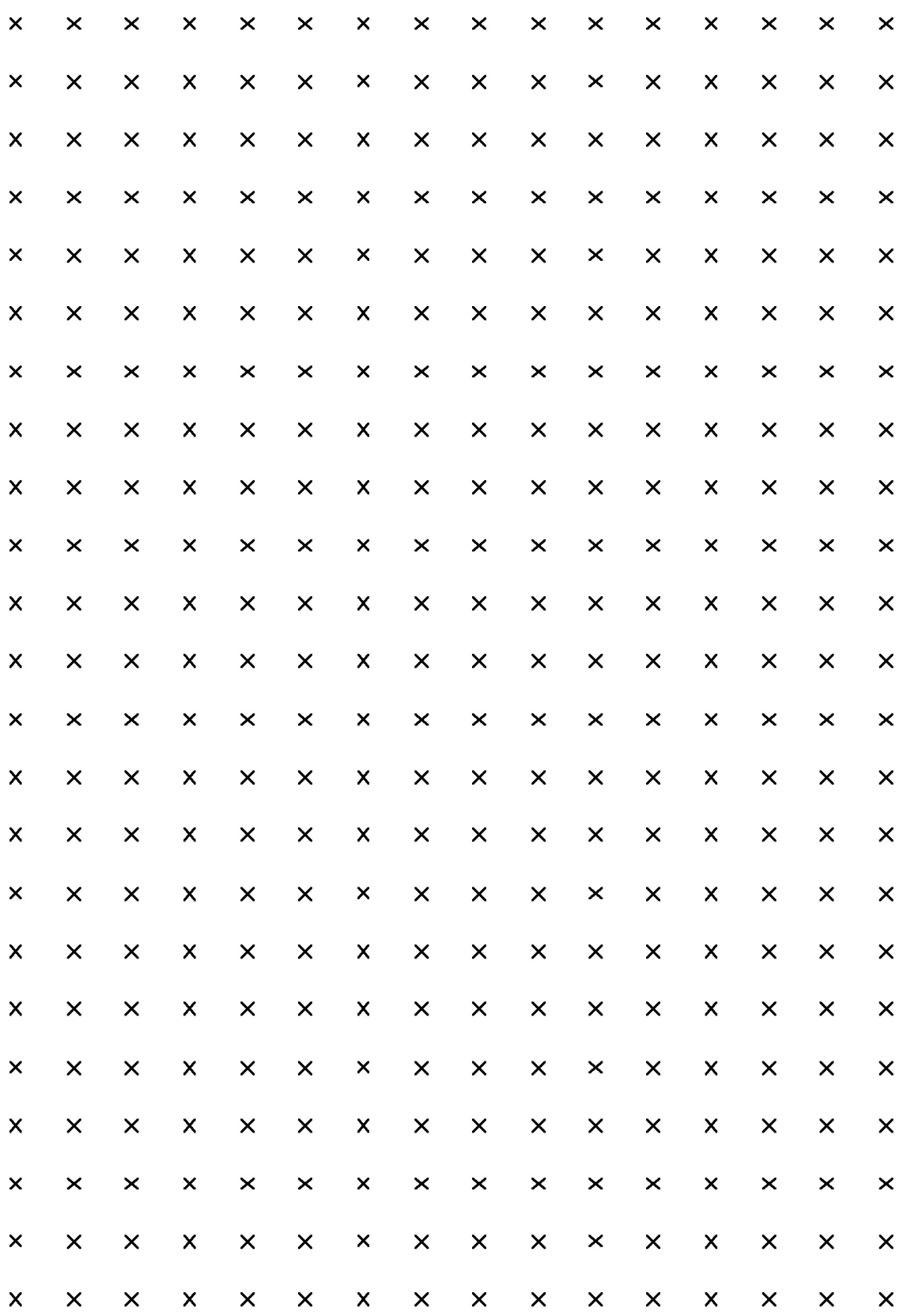

Figure 4: Template 2