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Group theory applied to crystallography

Solutions to the exercises

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Exercise 1.

In general, the product of affine mappings is not commutative, i.e. one usually has $\mathfrak{g} \cdot \mathfrak{h} \neq \mathfrak{h} \cdot \mathfrak{g}$. Prove that two affine mappings $\{g \mid t\}$ and $\{h \mid u\}$ commute if and only if

(i) the linear parts g and h commute;

(ii) the translation parts fulfill $(g - id) \cdot u = (h - id) \cdot t$.

Conclude that an arbitrary affine mapping $\{g \mid t\}$ commutes with a translation $\{id \mid u\}$ if and only if u is fixed under the action of g .

Solution: Writing out the products gives

$$\{g \mid t\} \cdot \{h \mid u\} = \{gh \mid g \cdot u + t\} \text{ and } \{h \mid u\} \cdot \{g \mid t\} = \{hg \mid h \cdot t + u\}.$$

These two elements are equal if their linear parts and their translation parts coincide, i.e. if $gh = hg$ and $g \cdot u + t = h \cdot t + u$ which is the same as $g \cdot u - u = h \cdot t - t$.

If $h = id$, then $h \cdot t - t = 0$, hence $g \cdot u - u$ has to be 0, i.e. $g \cdot u = u$.

Exercise 2.

Two space group elements are given by the following transformations:

$$\mathfrak{g} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} z + \frac{1}{2} \\ x + \frac{1}{2} \\ -y \end{pmatrix}, \quad \mathfrak{h} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -y \\ x + \frac{1}{2} \\ z + \frac{1}{2} \end{pmatrix}.$$

Determine the augmented matrices for \mathfrak{g} and \mathfrak{h} and compute the products $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$.

Solution: The augmented matrices are given by

$$\mathfrak{g} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & \frac{1}{2} \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} = \left(\begin{array}{ccc|c} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array} \right).$$

The products are

$$\mathfrak{g} \cdot \mathfrak{h} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & 1 \\ 0 & -1 & 0 & \frac{1}{2} \\ -1 & 0 & 0 & -\frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} \cdot \mathfrak{g} = \left(\begin{array}{ccc|c} -1 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & 1 \\ 0 & -1 & 0 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array} \right).$$

Exercise 3.

The point group P (in the geometric class $\bar{3}m1$) is generated by the matrices

$$g = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad h = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

- (i) Check that P fixes the metric tensor $F = \begin{pmatrix} 2a & -a & 0 \\ -a & 2a & 0 \\ 0 & 0 & b \end{pmatrix}$. It thus acts on a hexagonal lattice.
- (ii) P also acts on a rhombohedral lattice, which is obtained from the above hexagonal lattice by the basis transformation

$$X = \frac{1}{3} \begin{pmatrix} -1 & 2 & -1 \\ -2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \text{ with inverse transformation } X^{-1} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$

Transform the metric tensor F of the hexagonal lattice to the metric tensor of the rhombohedral lattice (with the columns of X as lattice basis).

- (iii) Transform P to the rhombohedral lattice (thus obtaining a point group P' in the arithmetic class $\bar{3}mR$) and check that the so obtained point group fixes the metric tensor computed in (ii).

Solution:

- (i) Check by matrix multiplication that indeed $g^{tr} F g = F$ and $h^{tr} F h = F$.
- (ii) Computing $F' = X^{tr} F X$ gives

$$F' = \frac{1}{9} \begin{pmatrix} 6a + b & -3a + b & -3a + b \\ -3a + b & 6a + b & -3a + b \\ -3a + b & -3a + b & 6a + b \end{pmatrix}.$$

- (iii) Computing $g' = X^{-1} g X$ and $h' = X^{-1} h X$ gives

$$g' = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \quad h' = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Now check that $g'^{tr} F' g' = F'$ and $h'^{tr} F' h' = F'$.

Exercise 4.

A space group G is generated by the elements

$$g = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{4} \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{array} \right), \quad h = \left(\begin{array}{cc|c} -1 & 0 & \frac{3}{2} \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{array} \right).$$

The point group P of G has 4 elements, the identity element and the linear parts of g , h and $g \cdot h$.

- (i) Determine the translation subgroup of G (which is not the standard lattice), transform G to a lattice basis of its translation lattice and write G in standard form. (Hint: g^2 and h^2 are translations.)

- (ii) The elements $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$ have the same linear part. Check that their translation part only differs by a lattice vector of the translation lattice.

Solution:

- (i) We have

$$\mathfrak{g}^2 = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h}^2 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{array} \right)$$

and $(\mathfrak{g} \cdot \mathfrak{h})^2$ is the identity element of G . A basis of the translation lattice is thus

$$\left(\begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right)$$

and with respect to this basis the four given generators become

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{cc|c} -1 & 0 & 3 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{array} \right).$$

In standard form, the group becomes the space group $\mathfrak{p}2\mathfrak{mg}$ given by the generators

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{array} \right).$$

- (ii) With respect to the original basis we have

$$\mathfrak{g} \cdot \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{7}{4} \\ 0 & -1 & -1 \\ 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} \cdot \mathfrak{g} = \left(\begin{array}{cc|c} -1 & 0 & \frac{5}{4} \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{array} \right),$$

the linear parts thus differ by

$$\begin{pmatrix} \frac{7}{4} \\ -1 \end{pmatrix} - \begin{pmatrix} \frac{5}{4} \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ -2 \end{pmatrix}$$

which is a lattice vector according to (i).

Exercise 5.

Show that an inner derivation $\{t_g = (g - id) \cdot v \mid g \in P\}$ fulfills the product condition $t_{gh} \equiv g \cdot t_h + t_g \pmod{L}$ by showing that even the equality $t_{gh} = g \cdot t_h + t_g$ holds.

Solution: We have $t_g = g \cdot v - v$, $t_h = h \cdot v - v$ and $t_{gh} = gh \cdot v - v$, thus

$$g \cdot t_h + t_g = gh \cdot v - g \cdot v + g \cdot v - v = gh \cdot v - v = t_{gh}.$$

Exercise 6.

Compute the inner derivations and the solutions of the Frobenius congruences modulo the inner derivations for the following point groups P :

(1) P is generated by

$$g = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, h = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$.

(2) P is generated by

$$g = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^4, y^2, (xy)^2 \rangle$.

Solution:

(1) Computing the inner derivation for $v = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ gives the inner derivation

$$\left(t_g = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, t_h = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \right),$$

computing the inner derivation for $v' = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ gives the inner derivation

$$\left(t'_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, t'_h = \begin{pmatrix} -2 \\ -2 \end{pmatrix} \right).$$

This shows that modulo inner derivations the first coordinate of t_g and the first coordinate of t_h can be chosen as 0.

We therefore insert the matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & a \\ 0 & 0 & 1 \end{array} \right), \mathfrak{h} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ -1 & 0 & b \\ 0 & 0 & 1 \end{array} \right)$$

into the relators, which yields

$$\mathfrak{g}^2 = \left(\begin{array}{cc|c} 1 & 0 & a \\ 0 & 1 & a \\ 0 & 0 & 1 \end{array} \right), \mathfrak{h}^2 = \left(\begin{array}{cc|c} 1 & 0 & -b \\ 0 & 1 & b \\ 0 & 0 & 1 \end{array} \right).$$

This implies $a = b = 0$, hence the only solutions to the Frobenius congruences are the inner derivations.

(2) The matrix $g - id$ is invertible, hence $(g - id) \cdot v$ runs over all vectors of \mathbb{R}^2 and we can thus assume that the SNoT element t_g of g is $t_g = 0$. We insert the matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right), \mathfrak{h} = \left(\begin{array}{cc|c} 1 & 0 & a \\ 0 & -1 & b \\ 0 & 0 & 1 \end{array} \right)$$

into the relators, which yields

$$\mathfrak{h}^2 = \left(\begin{array}{cc|c} 1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \quad (\mathfrak{gh})^2 = \left(\begin{array}{cc|c} 1 & 0 & a-b \\ 0 & 1 & a-b \\ 0 & 0 & 1 \end{array} \right).$$

The solutions of the Frobenius congruences modulo the inner derivations are thus $a = b = 0$ and $a = b = \frac{1}{2}$.

Exercise 7.

A certain point group P (known as $\overline{\mathfrak{m}3}$) is generated by

$$g = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \quad h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^6, y^2, (xy)^3, (x^3y)^2 \rangle$.

Since $g - id$ is invertible, $(g - id) \cdot v$ runs over all vectors in \mathbb{R}^3 , hence by a shift of origin the translation part of g may be assumed to be 0.

The integral normalizer of P contains the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ which interchanges the second and third basis vector.

Determine the solutions of the Frobenius congruences for P (assuming that $t_g = 0$) and check which of the resulting SNoTs lie in one orbit under the integral normalizer of P .

Solution: We insert the matrices

$$\mathfrak{g} = \left(\begin{array}{ccc|c} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} = \left(\begin{array}{ccc|c} -1 & 0 & 0 & a \\ 0 & 1 & 0 & b \\ 0 & 0 & 1 & c \\ 0 & 0 & 0 & 1 \end{array} \right),$$

into the relators, this gives

$$\mathfrak{h}^2 = \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2b \\ 0 & 0 & 1 & 2c \\ 0 & 0 & 0 & 1 \end{array} \right), \quad (\mathfrak{gh})^3 = \left(\begin{array}{ccc|c} 1 & 0 & 0 & a-b-c \\ 0 & 1 & 0 & -a+b+c \\ 0 & 0 & 1 & a-b-c \\ 0 & 0 & 0 & 1 \end{array} \right),$$

$$(\mathfrak{g}^3\mathfrak{h})^2 = \left(\begin{array}{ccc|c} 1 & 0 & 0 & -2a \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right)$$

The solutions to the Frobenius congruences are thus $a = b = c = 0$ and $a, b, c \in \{0, \frac{1}{2}\}$ with $a + b + c = 1$ and give rise to the four SNoTs

$$t_h^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad t_h^{(2)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \quad t_h^{(3)} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}, \quad t_h^{(4)} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

Conjugation of h with the normalizer element $a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ gives $a^{-1}ha = h$, thus only the action of a on the SNoT vectors t_h has to be considered. One sees that $t_h^{(1)}$ and $t_h^{(4)}$ are fixed under the action of a , but that $t_h^{(2)}$ and $t_h^{(3)}$ are interchanged and give thus rise to the same space group.

Exercise 8.

Let G be the space group of type p4gm generated as above by the matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & 1 \end{array} \right)$$

and the translations of the standard lattice. Let $x = \begin{pmatrix} 0.2 \\ 0.7 \end{pmatrix}$ be a point in the unit cell.

- (i) Determine the site-symmetry group G_x of x in G and show that it has point group type m .
- (ii) Find the points in the unit cell that lie in the orbit of x under G . (Hint: Since the point group P of G has order 8 and $|G_x| = 2$, you should find 4 points.)
- (iii) Find elements of G mapping x to each of the other three orbit points in the unit cell and determine the site-symmetry groups of these points.

Solution:

- (i) For an arbitrary element $\mathfrak{g} \in G$ the coset $T\mathfrak{g}$ contains an element of G_x if $\mathfrak{g}(x) - x$ is a lattice vector. We first apply \mathfrak{g} , \mathfrak{g}^2 and \mathfrak{g}^3 to x , this gives

$$\mathfrak{g}(x) = \begin{pmatrix} -0.7 \\ 0.2 \end{pmatrix}, \quad \mathfrak{g}^2(x) = \begin{pmatrix} -0.2 \\ -0.7 \end{pmatrix}, \quad \mathfrak{g}^3(x) = \begin{pmatrix} 0.7 \\ -0.2 \end{pmatrix}$$

and we see that none of these points differs by x by an integral vector in \mathbb{Z}^2 .

To cover all cosets, we now apply \mathfrak{h} to x , $\mathfrak{g}(x)$, $\mathfrak{g}^2(x)$, $\mathfrak{g}^3(x)$, this gives

$$\mathfrak{h}(x) = \begin{pmatrix} 0.3 \\ 1.2 \end{pmatrix}, \quad \mathfrak{h}\mathfrak{g}(x) = \begin{pmatrix} 1.2 \\ 0.7 \end{pmatrix}, \quad \mathfrak{h}\mathfrak{g}^2(x) = \begin{pmatrix} 0.7 \\ -0.2 \end{pmatrix}, \quad \mathfrak{h}\mathfrak{g}^3(x) = \begin{pmatrix} -0.2 \\ 0.3 \end{pmatrix}.$$

We see that the only case in which the orbit point differs from x by an integral vector is $\mathfrak{h}\mathfrak{g}(x) - x = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, hence G_x is generated by the reflection

$$\mathfrak{m} = \left(\begin{array}{cc|c} 0 & 1 & -\frac{1}{2} \\ 1 & 0 & \frac{1}{2} \\ 0 & 0 & 1 \end{array} \right).$$

- (ii) We only have to translate the orbit points found in (i) into the unit cell by suitable lattice vectors. This means to subtract the integer part from each of the coordinates. We obtain every point twice, the different points are

$$x_1 = x = \begin{pmatrix} 0.2 \\ 0.7 \end{pmatrix}, \quad x_2 = \begin{pmatrix} 0.3 \\ 0.2 \end{pmatrix}, \quad x_3 = \begin{pmatrix} 0.8 \\ 0.3 \end{pmatrix}, \quad x_4 = \begin{pmatrix} 0.7 \\ 0.8 \end{pmatrix}.$$

- (iii) We have actually obtained the points in the unit cell by applying the powers of \mathbf{g} and translating with a suitable lattice vector. If we call the vectors of the standard basis of \mathbb{Z}^2 (as usually) e_1 and e_2 , then we have $x_2 = \mathbf{g}(x) + e_1$, $x_3 = \mathbf{g}^2(x) + e_1 + e_2$, $x_4 = \mathbf{g}^3 + e_2$.

We now obtain the generators \mathbf{m}_2 , \mathbf{m}_3 and \mathbf{m}_4 for the site-symmetry groups of x_2 , x_3 and x_4 as the conjugates $\mathbf{g}_i \mathbf{m} \mathbf{g}_i^{-1}$ of \mathbf{m} by the corresponding augmented matrices

$$\mathbf{g}_2 = \left(\begin{array}{cc|c} 0 & -1 & 1 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \mathbf{g}_3 = \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & -1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \mathbf{g}_4 = \left(\begin{array}{cc|c} 0 & 1 & 0 \\ -1 & 0 & 1 \\ \hline 0 & 0 & 1 \end{array} \right).$$

Working this out gives the site-symmetry group generators

$$\mathbf{m}_2 = \left(\begin{array}{cc|c} 0 & -1 & \frac{1}{2} \\ -1 & 0 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right), \quad \mathbf{m}_3 = \left(\begin{array}{cc|c} 0 & 1 & \frac{1}{2} \\ 1 & 0 & -\frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right), \quad \mathbf{m}_4 = \left(\begin{array}{cc|c} 0 & -1 & \frac{3}{2} \\ -1 & 0 & \frac{3}{2} \\ \hline 0 & 0 & 1 \end{array} \right).$$

Exercise 9.

Let G be the space group of type $p2gg$ generated by the augmented matrices

$$\left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right).$$

Show that there are two Wyckoff positions of type 2 and that these Wyckoff positions belong to a single Wyckoff set. (Hint: It is enough to determine the translation part of the affine normalizer of G .)

Solution: Since the type of the site-symmetry group is requested to be 2, the generator of the site-symmetry group is necessarily of the form

$$\mathbf{g} = \left(\begin{array}{cc|c} -1 & 0 & a \\ 0 & -1 & b \\ \hline 0 & 0 & 1 \end{array} \right) \text{ with } a, b \in \mathbb{Z}.$$

Applying \mathbf{g} to the point $\begin{pmatrix} x \\ y \end{pmatrix}$ gives $\begin{pmatrix} -x + a \\ -y + b \end{pmatrix}$ and hence this point is fixed under \mathbf{g} if $-x + a = x$ and $-y + b = y$, i.e. if $2x = a$ and $2y = b$. Since we only have to consider points in the unit cell, we have on the one hand $0 \leq x, y < 1$ and on the other hand $a, b \in \mathbb{Z}$, hence $x, y \in \{0, \frac{1}{2}\}$. The positions with site-symmetry group of type 2 are thus

$$x_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad x_2 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \quad x_3 = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}, \quad x_4 = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}.$$

By applying one of the given generators of G we see that x_1 and x_4 lie in one orbit under G and also x_2 and x_3 lie in one orbit. On the other hand, x_1 and x_2 do not lie in one orbit, since the orbit of x_1 just consists of the lattice points and of the centers of the translates of the unit cell. Hence there are two Wyckoff positions with site-symmetry group of type 2.

In order to show that the two Wyckoff positions belong to the same Wyckoff set, we have to show that x_1 and x_2 lie in one orbit under the affine normalizer of G . The first guess is that the translation vector $v = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$ moving x_1 to x_2 lies in the normalizer. For that we have to check that $g \cdot v - v$ lies in the translation lattice for the linear parts g of the generators of G . We have

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \cdot v - v = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot v - v = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

hence the translation by v is indeed contained in the affine normalizer and thus x_1 and x_2 belong to the same Wyckoff set.