Exercise: Derivation of the space groups of a crystal class from the principles underlying the Hermann-Mauguin Symbols.

**Solution.** Determination of the space-group types of the crystal class $4/m \sim C_{4h}$ of order 8.

1. The two elements 4 and $m$ generate the group $4/m$.

2. The conventional setting is $4_z$ and $m_z$ in the tetragonal basis. The matrices of the generators $4_z$ and $m_z$ of $4/m$ are then

$$4_z = \begin{pmatrix} 0 & T & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad m_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & T \end{pmatrix}.$$

3. The matrices of the elements of $4/m$ are:

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad 4_z = \begin{pmatrix} 0 & T & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad 4_z^2 = 2_z = \begin{pmatrix} T & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad 4_z^4 = \begin{pmatrix} 0 & 1 & 0 \\ T & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

$$m_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad m_z * 4_z = 4_z^3 = \begin{pmatrix} 0 & T & 0 \\ 1 & 0 & 0 \\ 0 & 0 & T \end{pmatrix};$$

$$m_z * 2_z = 7 = \begin{pmatrix} T & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad m_z * 4_z^3 = 4_z = \begin{pmatrix} 0 & 1 & 0 \\ T & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

4. The most convenient origin is placed on the intersection of the $4_z$ axis with the plane $m_z$. The general $(4 \times 4)$-matrices of the corresponding generators of the space groups are then:

$$4_z = \begin{pmatrix} 0 & T & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \gamma \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad m_z = \begin{pmatrix} 1 & 0 & 0 & \alpha \\ 0 & 1 & 0 & \beta \\ 0 & 0 & T & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$
5. The compatibility conditions impose restrictions on the column coefficients:

(a) the reflection applied twice must result in a translation;
(b) the four-fold rotation applied four times must result in a translation;
(c) the first generator $4_z$ must be transformed by the second generator into an element of the group of $4_z$: $m_z^{-1} * 4_z * m_z = 4_z$.

For the unknown translation coefficients this means

(a) $\alpha = 0$ or $1/2$; $\beta = 0$ or $1/2$;
(b) $\gamma = k/4$ with $k = 0, 1, 2$, or $3$;
(c) the column $(-\alpha - \beta, \alpha - \beta, -k/2)$ must be a column of a translation of the lattice.

6. For the tetragonal $P$ lattice all lattice vectors have integer coefficients. Therefore, the coefficients $\alpha$ and $\beta$ must be both either $0$ or $1/2$ simultaneously, i.e. the reflection of the point group can only become a real reflection $m$ or an $n$-glide reflection in the space group. Independently, the coefficient $k$ is $0$ or $2$.

There are four space-group types:

$P4/m; P4_2/m, P4/n$ and $P4_2/n$.

7. The translation with the coefficients $(1/2, 1/2, 1/2)$ occurs in the tetragonal $I$ lattice. The four space-group types with the $P$ lattice merge into one type $I4/m$, because the four-fold rotation axes interchange with parallel $4_2$ screw rotation axes, whereas the $m$ reflection planes interchange with $n$ glide-reflection planes. However, now the combination $\alpha = 1/2$, $\beta = 0$, $k = 1$ is possible and results in the space-group type $I4_1/a$. Again, the other combinations: $b$-glide reflection and/or $4_3$ axes are equivalent and can be interpreted simply as the choices of other origins.

8. Altogether there belong six space-group types to the crystal class $4/m$:

$P4/m \sim C_{4h}^1$, No. 83; $P4_2/m \sim C_{4h}^2$, No. 84; $P4/n \sim C_{4h}^3$, No.85;

$P4_2/n \sim C_{4h}^4$, No. 86; $I4/m \sim C_{4h}^5$, No. 87 and $I4_1/a \sim C_{4h}^6$, No. 88.