

SG No. 193  $D_{6h}^3$   $P6_3/mcm$  [ hexagonal ]

\* plus set:  $+ [0, 0, 0]$

\* Wyckoff site: 2a, site symmetry:  $-62m$

Table 1: Wyckoff bond: 2a@2a

| No. | vector      | center                | mapping   |
|-----|-------------|-----------------------|---|
| 1   | $[0, 0, Z]$ | $[0, 0, \frac{1}{4}]$ | $[1, 2, 3, -7, -8, -9, -16, -17, -18, 22, 23, 24]$    |
| 2   | $[0, 0, Z]$ | $[0, 0, \frac{3}{4}]$ | $[4, 5, 6, -10, -11, -12, -13, -14, -15, 19, 20, 21]$ |

Table 2: Wyckoff bond: 6b@2a

| No. | vector         | center                | mapping             |
|-----|----------------|-----------------------|---------------------|
| 1   | $[X, 2X, 0]$   | $[0, 0, \frac{1}{4}]$ | $[1, -8, 16, -23]$  |
| 2   | $[-2X, -X, 0]$ | $[0, 0, \frac{1}{4}]$ | $[2, -7, 17, -22]$  |
| 3   | $[X, -X, 0]$   | $[0, 0, \frac{1}{4}]$ | $[3, -9, 18, -24]$  |
| 4   | $[-X, -2X, 0]$ | $[0, 0, \frac{3}{4}]$ | $[4, -11, 13, -20]$ |
| 5   | $[2X, X, 0]$   | $[0, 0, \frac{3}{4}]$ | $[5, -10, 14, -19]$ |
| 6   | $[-X, X, 0]$   | $[0, 0, \frac{3}{4}]$ | $[6, -12, 15, -21]$ |

Table 3: Wyckoff bond: 6c@2a

| No. | vector        | center                | mapping           |
|-----|---------------|-----------------------|-------------------|
| 1   | $[X, 0, 0]$   | $[0, 0, \frac{1}{4}]$ | $[1, 8, 16, 23]$  |
| 2   | $[0, X, 0]$   | $[0, 0, \frac{1}{4}]$ | $[2, 7, 17, 22]$  |
| 3   | $[-X, -X, 0]$ | $[0, 0, \frac{1}{4}]$ | $[3, 9, 18, 24]$  |
| 4   | $[-X, 0, 0]$  | $[0, 0, \frac{3}{4}]$ | $[4, 11, 13, 20]$ |
| 5   | $[0, -X, 0]$  | $[0, 0, \frac{3}{4}]$ | $[5, 10, 14, 19]$ |
| 6   | $[X, X, 0]$   | $[0, 0, \frac{3}{4}]$ | $[6, 12, 15, 21]$ |

Table 4: Wyckoff bond: 12d@2a

| No. | vector            | center                | mapping   |
|-----|-------------------|-----------------------|-----------|
| 1   | $[X, Y, 0]$       | $[0, 0, \frac{1}{4}]$ | $[1, 16]$ |
| 2   | $[-Y, X - Y, 0]$  | $[0, 0, \frac{1}{4}]$ | $[2, 17]$ |
| 3   | $[-X + Y, -X, 0]$ | $[0, 0, \frac{1}{4}]$ | $[3, 18]$ |
| 4   | $[-X, -Y, 0]$     | $[0, 0, \frac{3}{4}]$ | $[4, 13]$ |
| 5   | $[Y, -X + Y, 0]$  | $[0, 0, \frac{3}{4}]$ | $[5, 14]$ |
| 6   | $[X - Y, X, 0]$   | $[0, 0, \frac{3}{4}]$ | $[6, 15]$ |
| 7   | $[Y, X, 0]$       | $[0, 0, \frac{1}{4}]$ | $[7, 22]$ |
| 8   | $[X - Y, -Y, 0]$  | $[0, 0, \frac{1}{4}]$ | $[8, 23]$ |
| 9   | $[-X, -X + Y, 0]$ | $[0, 0, \frac{1}{4}]$ | $[9, 24]$ |

*continued ...*

Table 4

| No. | vector           | center                | mapping |
|-----|------------------|-----------------------|---------|
| 10  | $[-Y, -X, 0]$    | $[0, 0, \frac{3}{4}]$ | [10,19] |
| 11  | $[-X + Y, Y, 0]$ | $[0, 0, \frac{3}{4}]$ | [11,20] |
| 12  | $[X, X - Y, 0]$  | $[0, 0, \frac{3}{4}]$ | [12,21] |

Table 5: Wyckoff bond: 12e@2a

| No. | vector          | center                | mapping  |
|-----|-----------------|-----------------------|----------|
| 1   | $[X, 2X, Z]$    | $[0, 0, \frac{1}{4}]$ | [1,-8]   |
| 2   | $[-2X, -X, Z]$  | $[0, 0, \frac{1}{4}]$ | [2,-7]   |
| 3   | $[X, -X, Z]$    | $[0, 0, \frac{1}{4}]$ | [3,-9]   |
| 4   | $[-X, -2X, Z]$  | $[0, 0, \frac{3}{4}]$ | [4,-11]  |
| 5   | $[2X, X, Z]$    | $[0, 0, \frac{3}{4}]$ | [5,-10]  |
| 6   | $[-X, X, Z]$    | $[0, 0, \frac{3}{4}]$ | [6,-12]  |
| 7   | $[-X, -2X, -Z]$ | $[0, 0, \frac{3}{4}]$ | [13,-20] |
| 8   | $[2X, X, -Z]$   | $[0, 0, \frac{3}{4}]$ | [14,-19] |
| 9   | $[-X, X, -Z]$   | $[0, 0, \frac{3}{4}]$ | [15,-21] |
| 10  | $[X, 2X, -Z]$   | $[0, 0, \frac{1}{4}]$ | [16,-23] |
| 11  | $[-2X, -X, -Z]$ | $[0, 0, \frac{1}{4}]$ | [17,-22] |
| 12  | $[X, -X, -Z]$   | $[0, 0, \frac{1}{4}]$ | [18,-24] |

Table 6: Wyckoff bond: 12f@2a

| No. | vector         | center                | mapping |
|-----|----------------|-----------------------|---------|
| 1   | $[X, 0, Z]$    | $[0, 0, \frac{1}{4}]$ | [1,23]  |
| 2   | $[0, X, Z]$    | $[0, 0, \frac{1}{4}]$ | [2,22]  |
| 3   | $[-X, -X, Z]$  | $[0, 0, \frac{1}{4}]$ | [3,24]  |
| 4   | $[-X, 0, Z]$   | $[0, 0, \frac{3}{4}]$ | [4,20]  |
| 5   | $[0, -X, Z]$   | $[0, 0, \frac{3}{4}]$ | [5,19]  |
| 6   | $[X, X, Z]$    | $[0, 0, \frac{3}{4}]$ | [6,21]  |
| 7   | $[0, X, -Z]$   | $[0, 0, \frac{1}{4}]$ | [7,17]  |
| 8   | $[X, 0, -Z]$   | $[0, 0, \frac{1}{4}]$ | [8,16]  |
| 9   | $[-X, -X, -Z]$ | $[0, 0, \frac{1}{4}]$ | [9,18]  |
| 10  | $[0, -X, -Z]$  | $[0, 0, \frac{3}{4}]$ | [10,14] |
| 11  | $[-X, 0, -Z]$  | $[0, 0, \frac{3}{4}]$ | [11,13] |
| 12  | $[X, X, -Z]$   | $[0, 0, \frac{3}{4}]$ | [12,15] |

Table 7: Wyckoff bond: 24g@2a

| No. | vector             | center                | mapping |
|-----|--------------------|-----------------------|---------|
| 1   | $[X, Y, Z]$        | $[0, 0, \frac{1}{4}]$ | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[0, 0, \frac{1}{4}]$ | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[0, 0, \frac{1}{4}]$ | [3]     |
| 4   | $[-X, -Y, Z]$      | $[0, 0, \frac{3}{4}]$ | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[0, 0, \frac{3}{4}]$ | [5]     |
| 6   | $[X - Y, X, Z]$    | $[0, 0, \frac{3}{4}]$ | [6]     |
| 7   | $[Y, X, -Z]$       | $[0, 0, \frac{1}{4}]$ | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[0, 0, \frac{1}{4}]$ | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[0, 0, \frac{1}{4}]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[0, 0, \frac{3}{4}]$ | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[0, 0, \frac{3}{4}]$ | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[0, 0, \frac{3}{4}]$ | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[0, 0, \frac{3}{4}]$ | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[0, 0, \frac{3}{4}]$ | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[0, 0, \frac{3}{4}]$ | [15]    |
| 16  | $[X, Y, -Z]$       | $[0, 0, \frac{1}{4}]$ | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[0, 0, \frac{1}{4}]$ | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[0, 0, \frac{1}{4}]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[0, 0, \frac{3}{4}]$ | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[0, 0, \frac{3}{4}]$ | [20]    |
| 21  | $[X, X - Y, Z]$    | $[0, 0, \frac{3}{4}]$ | [21]    |
| 22  | $[Y, X, Z]$        | $[0, 0, \frac{1}{4}]$ | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[0, 0, \frac{1}{4}]$ | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[0, 0, \frac{1}{4}]$ | [24]    |

\* Wyckoff site: 2b, site symmetry:  $-3.m$

Table 8: Wyckoff bond: 2a@2b

| No. | vector      | center                | mapping   |
|-----|-------------|-----------------------|---|
| 1   | $[0, 0, Z]$ | $[0, 0, 0]$           | $[1, 2, 3, -10, -11, -12, -13, -14, -15, 22, 23, 24]$ |
| 2   | $[0, 0, Z]$ | $[0, 0, \frac{1}{2}]$ | $[4, 5, 6, -7, -8, -9, -16, -17, -18, 19, 20, 21]$    |

Table 9: Wyckoff bond: 6b@2b

| No. | vector        | center                | mapping             |
|-----|---------------|-----------------------|---------------------|
| 1   | $[X, 0, Z]$   | $[0, 0, 0]$           | $[1, -11, -13, 23]$ |
| 2   | $[0, X, Z]$   | $[0, 0, 0]$           | $[2, -10, -14, 22]$ |
| 3   | $[-X, -X, Z]$ | $[0, 0, 0]$           | $[3, -12, -15, 24]$ |
| 4   | $[-X, 0, Z]$  | $[0, 0, \frac{1}{2}]$ | $[4, -8, -16, 20]$  |
| 5   | $[0, -X, Z]$  | $[0, 0, \frac{1}{2}]$ | $[5, -7, -17, 19]$  |
| 6   | $[X, X, Z]$   | $[0, 0, \frac{1}{2}]$ | $[6, -9, -18, 21]$  |

Table 10: Wyckoff bond: 6c@2b

| No. | vector         | center                | mapping             |
|-----|----------------|-----------------------|---------------------|
| 1   | $[X, 2X, 0]$   | $[0, 0, 0]$           | $[1, 11, -13, -23]$ |
| 2   | $[-2X, -X, 0]$ | $[0, 0, 0]$           | $[2, 10, -14, -22]$ |
| 3   | $[X, -X, 0]$   | $[0, 0, 0]$           | $[3, 12, -15, -24]$ |
| 4   | $[-X, -2X, 0]$ | $[0, 0, \frac{1}{2}]$ | $[4, 8, -16, -20]$  |
| 5   | $[2X, X, 0]$   | $[0, 0, \frac{1}{2}]$ | $[5, 7, -17, -19]$  |
| 6   | $[-X, X, 0]$   | $[0, 0, \frac{1}{2}]$ | $[6, 9, -18, -21]$  |

Table 11: Wyckoff bond: 12d@2b

| No. | vector             | center                | mapping     |
|-----|--------------------|-----------------------|-------------|
| 1   | $[X, Y, Z]$        | $[0, 0, 0]$           | $[1, -13]$  |
| 2   | $[-Y, X - Y, Z]$   | $[0, 0, 0]$           | $[2, -14]$  |
| 3   | $[-X + Y, -X, Z]$  | $[0, 0, 0]$           | $[3, -15]$  |
| 4   | $[-X, -Y, Z]$      | $[0, 0, \frac{1}{2}]$ | $[4, -16]$  |
| 5   | $[Y, -X + Y, Z]$   | $[0, 0, \frac{1}{2}]$ | $[5, -17]$  |
| 6   | $[X - Y, X, Z]$    | $[0, 0, \frac{1}{2}]$ | $[6, -18]$  |
| 7   | $[Y, X, -Z]$       | $[0, 0, \frac{1}{2}]$ | $[7, -19]$  |
| 8   | $[X - Y, -Y, -Z]$  | $[0, 0, \frac{1}{2}]$ | $[8, -20]$  |
| 9   | $[-X, -X + Y, -Z]$ | $[0, 0, \frac{1}{2}]$ | $[9, -21]$  |
| 10  | $[-Y, -X, -Z]$     | $[0, 0, 0]$           | $[10, -22]$ |
| 11  | $[-X + Y, Y, -Z]$  | $[0, 0, 0]$           | $[11, -23]$ |
| 12  | $[X, X - Y, -Z]$   | $[0, 0, 0]$           | $[12, -24]$ |

\* Wyckoff site: 4c, site symmetry:  $-6..$

Table 12: Wyckoff bond: 4a@4c

| No. | vector       | center                                    | mapping                       |
|-----|--------------|---|-------------------------------|
| 1   | $[0, 0, Z]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | $[1, 2, 3, -16, -17, -18]$    |
| 2   | $[0, 0, Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | $[4, 5, 6, -13, -14, -15]$    |
| 3   | $[0, 0, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | $[7, 8, 9, -22, -23, -24]$    |
| 4   | $[0, 0, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | $[10, 11, 12, -19, -20, -21]$ |

Table 13: Wyckoff bond: 12b@4c

| No. | vector           | center                                    | mapping   |
|-----|------------------|---|-----------|
| 1   | $[X, Y, 0]$      | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | $[1, 16]$ |
| 2   | $[-Y, X - Y, 0]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | $[2, 17]$ |

*continued ...*

Table 13

| No. | vector            | center                                    | mapping  |
|-----|-------------------|---|----------|
| 3   | $[-X + Y, -X, 0]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [3, 18]  |
| 4   | $[-X, -Y, 0]$     | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [4, 13]  |
| 5   | $[Y, -X + Y, 0]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [5, 14]  |
| 6   | $[X - Y, X, 0]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [6, 15]  |
| 7   | $[Y, X, 0]$       | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [7, 22]  |
| 8   | $[X - Y, -Y, 0]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [8, 23]  |
| 9   | $[-X, -X + Y, 0]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [9, 24]  |
| 10  | $[-Y, -X, 0]$     | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [10, 19] |
| 11  | $[-X + Y, Y, 0]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [11, 20] |
| 12  | $[X, X - Y, 0]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [12, 21] |

Table 14: Wyckoff bond: 24c@4c

| No. | vector             | center                                    | mapping |
|-----|--------------------|---|---------|
| 1   | $[X, Y, Z]$        | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [3]     |
| 4   | $[-X, -Y, Z]$      | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [5]     |
| 6   | $[X - Y, X, Z]$    | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [6]     |
| 7   | $[Y, X, -Z]$       | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$ | [15]    |
| 16  | $[X, Y, -Z]$       | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [20]    |
| 21  | $[X, X - Y, Z]$    | $[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$ | [21]    |
| 22  | $[Y, X, Z]$        | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$ | [24]    |

\* Wyckoff site: 4d, site symmetry: 3.2

Table 15: Wyckoff bond: 4a@4d

| No. | vector       | center                                    | mapping                       |
|-----|--------------|---|-------------------------------|
| 1   | $[0, 0, Z]$  | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[1, 2, 3, -10, -11, -12]$    |
| 2   | $[0, 0, Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[4, 5, 6, -7, -8, -9]$       |
| 3   | $[0, 0, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[13, 14, 15, -22, -23, -24]$ |
| 4   | $[0, 0, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[16, 17, 18, -19, -20, -21]$ |

Table 16: Wyckoff bond: 12b@4d

| No. | vector         | center                                    | mapping     |
|-----|----------------|---|-------------|
| 1   | $[X, 0, Z]$    | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[1, -11]$  |
| 2   | $[0, X, Z]$    | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[2, -10]$  |
| 3   | $[-X, -X, Z]$  | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[3, -12]$  |
| 4   | $[-X, 0, Z]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[4, -8]$   |
| 5   | $[0, -X, Z]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[5, -7]$   |
| 6   | $[X, X, Z]$    | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[6, -9]$   |
| 7   | $[-X, 0, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[13, -23]$ |
| 8   | $[0, -X, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[14, -22]$ |
| 9   | $[X, X, -Z]$   | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[15, -24]$ |
| 10  | $[X, 0, -Z]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[16, -20]$ |
| 11  | $[0, X, -Z]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[17, -19]$ |
| 12  | $[-X, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[18, -21]$ |

Table 17: Wyckoff bond: 12c@4d

| No. | vector         | center                                    | mapping    |
|-----|----------------|---|------------|
| 1   | $[X, 2X, 0]$   | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[1, 11]$  |
| 2   | $[-2X, -X, 0]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[2, 10]$  |
| 3   | $[X, -X, 0]$   | $[\frac{1}{3}, \frac{2}{3}, 0]$           | $[3, 12]$  |
| 4   | $[-X, -2X, 0]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[4, 8]$   |
| 5   | $[2X, X, 0]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[5, 7]$   |
| 6   | $[-X, X, 0]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | $[6, 9]$   |
| 7   | $[-X, -2X, 0]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[13, 23]$ |
| 8   | $[2X, X, 0]$   | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[14, 22]$ |
| 9   | $[-X, X, 0]$   | $[\frac{2}{3}, \frac{1}{3}, 0]$           | $[15, 24]$ |
| 10  | $[X, 2X, 0]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[16, 20]$ |
| 11  | $[-2X, -X, 0]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[17, 19]$ |
| 12  | $[X, -X, 0]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | $[18, 21]$ |

Table 18: Wyckoff bond: 24d@4d

| No. | vector             | center                                    | mapping |
|-----|--------------------|---|---------|
| 1   | $[X, Y, Z]$        | $[\frac{1}{3}, \frac{2}{3}, 0]$           | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[\frac{1}{3}, \frac{2}{3}, 0]$           | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[\frac{1}{3}, \frac{2}{3}, 0]$           | [3]     |
| 4   | $[-X, -Y, Z]$      | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [5]     |
| 6   | $[X - Y, X, Z]$    | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [6]     |
| 7   | $[Y, X, -Z]$       | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[\frac{1}{3}, \frac{2}{3}, 0]$           | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[\frac{1}{3}, \frac{2}{3}, 0]$           | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[\frac{1}{3}, \frac{2}{3}, 0]$           | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[\frac{2}{3}, \frac{1}{3}, 0]$           | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, 0]$           | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[\frac{2}{3}, \frac{1}{3}, 0]$           | [15]    |
| 16  | $[X, Y, -Z]$       | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [20]    |
| 21  | $[X, X - Y, Z]$    | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [21]    |
| 22  | $[Y, X, Z]$        | $[\frac{2}{3}, \frac{1}{3}, 0]$           | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[\frac{2}{3}, \frac{1}{3}, 0]$           | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[\frac{2}{3}, \frac{1}{3}, 0]$           | [24]    |

\* Wyckoff site: 4e, site symmetry: 3.m

Table 19: Wyckoff bond: 4a@4e

| No. | vector       | center                    | mapping                  |
|-----|--------------|---------------------------|--------------------------|
| 1   | $[0, 0, Z]$  | $[0, 0, z]$               | [1, 2, 3, 22, 23, 24]    |
| 2   | $[0, 0, Z]$  | $[0, 0, z + \frac{1}{2}]$ | [4, 5, 6, 19, 20, 21]    |
| 3   | $[0, 0, -Z]$ | $[0, 0, \frac{1}{2} - z]$ | [7, 8, 9, 16, 17, 18]    |
| 4   | $[0, 0, -Z]$ | $[0, 0, -z]$              | [10, 11, 12, 13, 14, 15] |

Table 20: Wyckoff bond: 12b@4e

| No. | vector        | center                    | mapping |
|-----|---------------|---------------------------|---------|
| 1   | $[X, 0, Z]$   | $[0, 0, z]$               | [1, 23] |
| 2   | $[0, X, Z]$   | $[0, 0, z]$               | [2, 22] |
| 3   | $[-X, -X, Z]$ | $[0, 0, z]$               | [3, 24] |
| 4   | $[-X, 0, Z]$  | $[0, 0, z + \frac{1}{2}]$ | [4, 20] |

*continued ...*

Table 20

| No. | vector         | center                    | mapping |
|-----|----------------|---------------------------|---------|
| 5   | $[0, -X, Z]$   | $[0, 0, z + \frac{1}{2}]$ | [5,19]  |
| 6   | $[X, X, Z]$    | $[0, 0, z + \frac{1}{2}]$ | [6,21]  |
| 7   | $[0, X, -Z]$   | $[0, 0, \frac{1}{2} - z]$ | [7,17]  |
| 8   | $[X, 0, -Z]$   | $[0, 0, \frac{1}{2} - z]$ | [8,16]  |
| 9   | $[-X, -X, -Z]$ | $[0, 0, \frac{1}{2} - z]$ | [9,18]  |
| 10  | $[0, -X, -Z]$  | $[0, 0, -z]$              | [10,14] |
| 11  | $[-X, 0, -Z]$  | $[0, 0, -z]$              | [11,13] |
| 12  | $[X, X, -Z]$   | $[0, 0, -z]$              | [12,15] |

Table 21: Wyckoff bond: 12c@4e

| No. | vector         | center                    | mapping  |
|-----|----------------|---------------------------|----------|
| 1   | $[X, 2X, 0]$   | $[0, 0, z]$               | [1,-23]  |
| 2   | $[-2X, -X, 0]$ | $[0, 0, z]$               | [2,-22]  |
| 3   | $[X, -X, 0]$   | $[0, 0, z]$               | [3,-24]  |
| 4   | $[-X, -2X, 0]$ | $[0, 0, z + \frac{1}{2}]$ | [4,-20]  |
| 5   | $[2X, X, 0]$   | $[0, 0, z + \frac{1}{2}]$ | [5,-19]  |
| 6   | $[-X, X, 0]$   | $[0, 0, z + \frac{1}{2}]$ | [6,-21]  |
| 7   | $[2X, X, 0]$   | $[0, 0, \frac{1}{2} - z]$ | [7,-17]  |
| 8   | $[-X, -2X, 0]$ | $[0, 0, \frac{1}{2} - z]$ | [8,-16]  |
| 9   | $[-X, X, 0]$   | $[0, 0, \frac{1}{2} - z]$ | [9,-18]  |
| 10  | $[-2X, -X, 0]$ | $[0, 0, -z]$              | [10,-14] |
| 11  | $[X, 2X, 0]$   | $[0, 0, -z]$              | [11,-13] |
| 12  | $[X, -X, 0]$   | $[0, 0, -z]$              | [12,-15] |

Table 22: Wyckoff bond: 24d@4e

| No. | vector             | center                    | mapping |
|-----|--------------------|---------------------------|---------|
| 1   | $[X, Y, Z]$        | $[0, 0, z]$               | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[0, 0, z]$               | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[0, 0, z]$               | [3]     |
| 4   | $[-X, -Y, Z]$      | $[0, 0, z + \frac{1}{2}]$ | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[0, 0, z + \frac{1}{2}]$ | [5]     |
| 6   | $[X - Y, X, Z]$    | $[0, 0, z + \frac{1}{2}]$ | [6]     |
| 7   | $[Y, X, -Z]$       | $[0, 0, \frac{1}{2} - z]$ | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[0, 0, \frac{1}{2} - z]$ | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[0, 0, \frac{1}{2} - z]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[0, 0, -z]$              | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[0, 0, -z]$              | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[0, 0, -z]$              | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[0, 0, -z]$              | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[0, 0, -z]$              | [14]    |

*continued ...*

Table 22

| No. | vector             | center                    | mapping |
|-----|--------------------|---------------------------|---------|
| 15  | $[X - Y, X, -Z]$   | $[0, 0, -z]$              | [15]    |
| 16  | $[X, Y, -Z]$       | $[0, 0, \frac{1}{2} - z]$ | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[0, 0, \frac{1}{2} - z]$ | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[0, 0, \frac{1}{2} - z]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[0, 0, z + \frac{1}{2}]$ | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[0, 0, z + \frac{1}{2}]$ | [20]    |
| 21  | $[X, X - Y, Z]$    | $[0, 0, z + \frac{1}{2}]$ | [21]    |
| 22  | $[Y, X, Z]$        | $[0, 0, z]$               | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[0, 0, z]$               | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[0, 0, z]$               | [24]    |

\* Wyckoff site: 6f, site symmetry:  $\dots/m$

Table 23: Wyckoff bond: 6a@6f

| No. | vector        | center                                    | mapping           |
|-----|---------------|---|-------------------|
| 1   | $[X, 0, Z]$   | $[\frac{1}{2}, 0, 0]$                     | [1, -11, -13, 23] |
| 2   | $[0, X, Z]$   | $[0, \frac{1}{2}, 0]$                     | [2, -10, -14, 22] |
| 3   | $[-X, -X, Z]$ | $[\frac{1}{2}, \frac{1}{2}, 0]$           | [3, -12, -15, 24] |
| 4   | $[-X, 0, Z]$  | $[\frac{1}{2}, 0, \frac{1}{2}]$           | [4, -8, -16, 20]  |
| 5   | $[0, -X, Z]$  | $[0, \frac{1}{2}, \frac{1}{2}]$           | [5, -7, -17, 19]  |
| 6   | $[X, X, Z]$   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [6, -9, -18, 21]  |

Table 24: Wyckoff bond: 6b@6f

| No. | vector         | center                                    | mapping           |
|-----|----------------|---|-------------------|
| 1   | $[X, 2X, 0]$   | $[\frac{1}{2}, 0, 0]$                     | [1, 11, -13, -23] |
| 2   | $[-2X, -X, 0]$ | $[0, \frac{1}{2}, 0]$                     | [2, 10, -14, -22] |
| 3   | $[X, -X, 0]$   | $[\frac{1}{2}, \frac{1}{2}, 0]$           | [3, 12, -15, -24] |
| 4   | $[-X, -2X, 0]$ | $[\frac{1}{2}, 0, \frac{1}{2}]$           | [4, 8, -16, -20]  |
| 5   | $[2X, X, 0]$   | $[0, \frac{1}{2}, \frac{1}{2}]$           | [5, 7, -17, -19]  |
| 6   | $[-X, X, 0]$   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [6, 9, -18, -21]  |

Table 25: Wyckoff bond: 12c@6f

| No. | vector            | center                          | mapping  |
|-----|-------------------|---------------------------------|----------|
| 1   | $[X, Y, Z]$       | $[\frac{1}{2}, 0, 0]$           | [1, -13] |
| 2   | $[-Y, X - Y, Z]$  | $[0, \frac{1}{2}, 0]$           | [2, -14] |
| 3   | $[-X + Y, -X, Z]$ | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [3, -15] |
| 4   | $[-X, -Y, Z]$     | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [4, -16] |

*continued ...*

Table 25

| No. | vector             | center                                    | mapping   |
|-----|--------------------|---|-----------|
| 5   | $[Y, -X + Y, Z]$   | $[0, \frac{1}{2}, \frac{1}{2}]$           | [5, -17]  |
| 6   | $[X - Y, X, Z]$    | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [6, -18]  |
| 7   | $[Y, X, -Z]$       | $[0, \frac{1}{2}, \frac{1}{2}]$           | [7, -19]  |
| 8   | $[X - Y, -Y, -Z]$  | $[\frac{1}{2}, 0, \frac{1}{2}]$           | [8, -20]  |
| 9   | $[-X, -X + Y, -Z]$ | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [9, -21]  |
| 10  | $[-Y, -X, -Z]$     | $[0, \frac{1}{2}, 0]$                     | [10, -22] |
| 11  | $[-X + Y, Y, -Z]$  | $[\frac{1}{2}, 0, 0]$                     | [11, -23] |
| 12  | $[X, X - Y, -Z]$   | $[\frac{1}{2}, \frac{1}{2}, 0]$           | [12, -24] |

\* Wyckoff site: 6g, site symmetry: m2m

Table 26: Wyckoff bond: 6a@6g

| No. | vector         | center                  | mapping           |
|-----|----------------|-------------------------|-------------------|
| 1   | $[X, 2X, 0]$   | $[x, 0, \frac{1}{4}]$   | [1, -8, 16, -23]  |
| 2   | $[-2X, -X, 0]$ | $[0, x, \frac{1}{4}]$   | [2, -7, 17, -22]  |
| 3   | $[X, -X, 0]$   | $[-x, -x, \frac{1}{4}]$ | [3, -9, 18, -24]  |
| 4   | $[-X, -2X, 0]$ | $[-x, 0, \frac{3}{4}]$  | [4, -11, 13, -20] |
| 5   | $[2X, X, 0]$   | $[0, -x, \frac{3}{4}]$  | [5, -10, 14, -19] |
| 6   | $[-X, X, 0]$   | $[x, x, \frac{3}{4}]$   | [6, -12, 15, -21] |

Table 27: Wyckoff bond: 6b@6g

| No. | vector        | center                  | mapping         |
|-----|---------------|-------------------------|-----------------|
| 1   | $[X, 0, 0]$   | $[x, 0, \frac{1}{4}]$   | [1, 8, 16, 23]  |
| 2   | $[0, X, 0]$   | $[0, x, \frac{1}{4}]$   | [2, 7, 17, 22]  |
| 3   | $[-X, -X, 0]$ | $[-x, -x, \frac{1}{4}]$ | [3, 9, 18, 24]  |
| 4   | $[-X, 0, 0]$  | $[-x, 0, \frac{3}{4}]$  | [4, 11, 13, 20] |
| 5   | $[0, -X, 0]$  | $[0, -x, \frac{3}{4}]$  | [5, 10, 14, 19] |
| 6   | $[X, X, 0]$   | $[x, x, \frac{3}{4}]$   | [6, 12, 15, 21] |

Table 28: Wyckoff bond: 6c@6g

| No. | vector      | center                  | mapping           |
|-----|-------------|-------------------------|-------------------|
| 1   | $[0, 0, Z]$ | $[x, 0, \frac{1}{4}]$   | [1, -8, -16, 23]  |
| 2   | $[0, 0, Z]$ | $[0, x, \frac{1}{4}]$   | [2, -7, -17, 22]  |
| 3   | $[0, 0, Z]$ | $[-x, -x, \frac{1}{4}]$ | [3, -9, -18, 24]  |
| 4   | $[0, 0, Z]$ | $[-x, 0, \frac{3}{4}]$  | [4, -11, -13, 20] |
| 5   | $[0, 0, Z]$ | $[0, -x, \frac{3}{4}]$  | [5, -10, -14, 19] |
| 6   | $[0, 0, Z]$ | $[x, x, \frac{3}{4}]$   | [6, -12, -15, 21] |

Table 29: Wyckoff bond: 12d06g

| No. | vector            | center                  | mapping |
|-----|-------------------|-------------------------|---------|
| 1   | $[X, Y, 0]$       | $[x, 0, \frac{1}{4}]$   | [1,16]  |
| 2   | $[-Y, X - Y, 0]$  | $[0, x, \frac{1}{4}]$   | [2,17]  |
| 3   | $[-X + Y, -X, 0]$ | $[-x, -x, \frac{1}{4}]$ | [3,18]  |
| 4   | $[-X, -Y, 0]$     | $[-x, 0, \frac{3}{4}]$  | [4,13]  |
| 5   | $[Y, -X + Y, 0]$  | $[0, -x, \frac{3}{4}]$  | [5,14]  |
| 6   | $[X - Y, X, 0]$   | $[x, x, \frac{3}{4}]$   | [6,15]  |
| 7   | $[Y, X, 0]$       | $[0, x, \frac{1}{4}]$   | [7,22]  |
| 8   | $[X - Y, -Y, 0]$  | $[x, 0, \frac{1}{4}]$   | [8,23]  |
| 9   | $[-X, -X + Y, 0]$ | $[-x, -x, \frac{1}{4}]$ | [9,24]  |
| 10  | $[-Y, -X, 0]$     | $[0, -x, \frac{3}{4}]$  | [10,19] |
| 11  | $[-X + Y, Y, 0]$  | $[-x, 0, \frac{3}{4}]$  | [11,20] |
| 12  | $[X, X - Y, 0]$   | $[x, x, \frac{3}{4}]$   | [12,21] |

Table 30: Wyckoff bond: 12e06g

| No. | vector          | center                  | mapping  |
|-----|-----------------|-------------------------|----------|
| 1   | $[X, 2X, Z]$    | $[x, 0, \frac{1}{4}]$   | [1,-8]   |
| 2   | $[-2X, -X, Z]$  | $[0, x, \frac{1}{4}]$   | [2,-7]   |
| 3   | $[X, -X, Z]$    | $[-x, -x, \frac{1}{4}]$ | [3,-9]   |
| 4   | $[-X, -2X, Z]$  | $[-x, 0, \frac{3}{4}]$  | [4,-11]  |
| 5   | $[2X, X, Z]$    | $[0, -x, \frac{3}{4}]$  | [5,-10]  |
| 6   | $[-X, X, Z]$    | $[x, x, \frac{3}{4}]$   | [6,-12]  |
| 7   | $[-X, -2X, -Z]$ | $[-x, 0, \frac{3}{4}]$  | [13,-20] |
| 8   | $[2X, X, -Z]$   | $[0, -x, \frac{3}{4}]$  | [14,-19] |
| 9   | $[-X, X, -Z]$   | $[x, x, \frac{3}{4}]$   | [15,-21] |
| 10  | $[X, 2X, -Z]$   | $[x, 0, \frac{1}{4}]$   | [16,-23] |
| 11  | $[-2X, -X, -Z]$ | $[0, x, \frac{1}{4}]$   | [17,-22] |
| 12  | $[X, -X, -Z]$   | $[-x, -x, \frac{1}{4}]$ | [18,-24] |

Table 31: Wyckoff bond: 12f06g

| No. | vector        | center                  | mapping |
|-----|---------------|-------------------------|---------|
| 1   | $[X, 0, Z]$   | $[x, 0, \frac{1}{4}]$   | [1,23]  |
| 2   | $[0, X, Z]$   | $[0, x, \frac{1}{4}]$   | [2,22]  |
| 3   | $[-X, -X, Z]$ | $[-x, -x, \frac{1}{4}]$ | [3,24]  |
| 4   | $[-X, 0, Z]$  | $[-x, 0, \frac{3}{4}]$  | [4,20]  |
| 5   | $[0, -X, Z]$  | $[0, -x, \frac{3}{4}]$  | [5,19]  |
| 6   | $[X, X, Z]$   | $[x, x, \frac{3}{4}]$   | [6,21]  |
| 7   | $[0, X, -Z]$  | $[0, x, \frac{1}{4}]$   | [7,17]  |

continued ...

Table 31

| No. | vector         | center                  | mapping |
|-----|----------------|-------------------------|---------|
| 8   | $[X, 0, -Z]$   | $[x, 0, \frac{1}{4}]$   | [8,16]  |
| 9   | $[-X, -X, -Z]$ | $[-x, -x, \frac{1}{4}]$ | [9,18]  |
| 10  | $[0, -X, -Z]$  | $[0, -x, \frac{3}{4}]$  | [10,14] |
| 11  | $[-X, 0, -Z]$  | $[-x, 0, \frac{3}{4}]$  | [11,13] |
| 12  | $[X, X, -Z]$   | $[x, x, \frac{3}{4}]$   | [12,15] |

Table 32: Wyckoff bond: 24g@6g

| No. | vector             | center                  | mapping |
|-----|--------------------|-------------------------|---------|
| 1   | $[X, Y, Z]$        | $[x, 0, \frac{1}{4}]$   | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[0, x, \frac{1}{4}]$   | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[-x, -x, \frac{1}{4}]$ | [3]     |
| 4   | $[-X, -Y, Z]$      | $[-x, 0, \frac{3}{4}]$  | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[0, -x, \frac{3}{4}]$  | [5]     |
| 6   | $[X - Y, X, Z]$    | $[x, x, \frac{3}{4}]$   | [6]     |
| 7   | $[Y, X, -Z]$       | $[0, x, \frac{1}{4}]$   | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[x, 0, \frac{1}{4}]$   | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[-x, -x, \frac{1}{4}]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[0, -x, \frac{3}{4}]$  | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[-x, 0, \frac{3}{4}]$  | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[x, x, \frac{3}{4}]$   | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[-x, 0, \frac{3}{4}]$  | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[0, -x, \frac{3}{4}]$  | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[x, x, \frac{3}{4}]$   | [15]    |
| 16  | $[X, Y, -Z]$       | $[x, 0, \frac{1}{4}]$   | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[0, x, \frac{1}{4}]$   | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[-x, -x, \frac{1}{4}]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[0, -x, \frac{3}{4}]$  | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[-x, 0, \frac{3}{4}]$  | [20]    |
| 21  | $[X, X - Y, Z]$    | $[x, x, \frac{3}{4}]$   | [21]    |
| 22  | $[Y, X, Z]$        | $[0, x, \frac{1}{4}]$   | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[x, 0, \frac{1}{4}]$   | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[-x, -x, \frac{1}{4}]$ | [24]    |

\* Wyckoff site: 8h, site symmetry: 3..

Table 33: Wyckoff bond: 8a@8h

| No. | vector       | center  | mapping |
|-----|--------------|---|---------|
| 1   | $[0, 0, Z]$  | $[\frac{1}{3}, \frac{2}{3}, z]$               | [1,2,3] |
| 2   | $[0, 0, Z]$  | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [4,5,6] |
| 3   | $[0, 0, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$ | [7,8,9] |

continued ...

Table 33

| No. | vector       | center  | mapping      |
|-----|--------------|---|--------------|
| 4   | $[0, 0, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, -z]$              | [10, 11, 12] |
| 5   | $[0, 0, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$              | [13, 14, 15] |
| 6   | $[0, 0, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$ | [16, 17, 18] |
| 7   | $[0, 0, Z]$  | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$ | [19, 20, 21] |
| 8   | $[0, 0, Z]$  | $[\frac{2}{3}, \frac{1}{3}, z]$               | [22, 23, 24] |

Table 34: Wyckoff bond: 24b@8h

| No. | vector             | center  | mapping |
|-----|--------------------|---|---------|
| 1   | $[X, Y, Z]$        | $[\frac{1}{3}, \frac{2}{3}, z]$               | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[\frac{1}{3}, \frac{2}{3}, z]$               | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[\frac{1}{3}, \frac{2}{3}, z]$               | [3]     |
| 4   | $[-X, -Y, Z]$      | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [5]     |
| 6   | $[X - Y, X, Z]$    | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [6]     |
| 7   | $[Y, X, -Z]$       | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$ | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$ | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[\frac{1}{3}, \frac{2}{3}, -z]$              | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[\frac{1}{3}, \frac{2}{3}, -z]$              | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[\frac{1}{3}, \frac{2}{3}, -z]$              | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[\frac{2}{3}, \frac{1}{3}, -z]$              | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[\frac{2}{3}, \frac{1}{3}, -z]$              | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[\frac{2}{3}, \frac{1}{3}, -z]$              | [15]    |
| 16  | $[X, Y, -Z]$       | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$ | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$ | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$ | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$ | [20]    |
| 21  | $[X, X - Y, Z]$    | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$ | [21]    |
| 22  | $[Y, X, Z]$        | $[\frac{2}{3}, \frac{1}{3}, z]$               | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[\frac{2}{3}, \frac{1}{3}, z]$               | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[\frac{2}{3}, \frac{1}{3}, z]$               | [24]    |

\* Wyckoff site: 12i, site symmetry:  $\dots 2$

Table 35: Wyckoff bond: 12a@12i

| No. | vector        | center         | mapping  |
|-----|---------------|----------------|----------|
| 1   | $[X, 0, Z]$   | $[x, 2x, 0]$   | [1, -11] |
| 2   | $[0, X, Z]$   | $[-2x, -x, 0]$ | [2, -10] |
| 3   | $[-X, -X, Z]$ | $[x, -x, 0]$   | [3, -12] |

*continued ...*

Table 35

| No. | vector         | center                   | mapping  |
|-----|----------------|--------------------------|----------|
| 4   | $[-X, 0, Z]$   | $[-x, -2x, \frac{1}{2}]$ | [4,-8]   |
| 5   | $[0, -X, Z]$   | $[2x, x, \frac{1}{2}]$   | [5,-7]   |
| 6   | $[X, X, Z]$    | $[-x, x, \frac{1}{2}]$   | [6,-9]   |
| 7   | $[-X, 0, -Z]$  | $[-x, -2x, 0]$           | [13,-23] |
| 8   | $[0, -X, -Z]$  | $[2x, x, 0]$             | [14,-22] |
| 9   | $[X, X, -Z]$   | $[-x, x, 0]$             | [15,-24] |
| 10  | $[X, 0, -Z]$   | $[x, 2x, \frac{1}{2}]$   | [16,-20] |
| 11  | $[0, X, -Z]$   | $[-2x, -x, \frac{1}{2}]$ | [17,-19] |
| 12  | $[-X, -X, -Z]$ | $[x, -x, \frac{1}{2}]$   | [18,-21] |

Table 36: Wyckoff bond: 12b@12i

| No. | vector         | center                   | mapping |
|-----|----------------|--------------------------|---------|
| 1   | $[X, 2X, 0]$   | $[x, 2x, 0]$             | [1,11]  |
| 2   | $[-2X, -X, 0]$ | $[-2x, -x, 0]$           | [2,10]  |
| 3   | $[X, -X, 0]$   | $[x, -x, 0]$             | [3,12]  |
| 4   | $[-X, -2X, 0]$ | $[-x, -2x, \frac{1}{2}]$ | [4,8]   |
| 5   | $[2X, X, 0]$   | $[2x, x, \frac{1}{2}]$   | [5,7]   |
| 6   | $[-X, X, 0]$   | $[-x, x, \frac{1}{2}]$   | [6,9]   |
| 7   | $[-X, -2X, 0]$ | $[-x, -2x, 0]$           | [13,23] |
| 8   | $[2X, X, 0]$   | $[2x, x, 0]$             | [14,22] |
| 9   | $[-X, X, 0]$   | $[-x, x, 0]$             | [15,24] |
| 10  | $[X, 2X, 0]$   | $[x, 2x, \frac{1}{2}]$   | [16,20] |
| 11  | $[-2X, -X, 0]$ | $[-2x, -x, \frac{1}{2}]$ | [17,19] |
| 12  | $[X, -X, 0]$   | $[x, -x, \frac{1}{2}]$   | [18,21] |

Table 37: Wyckoff bond: 24c@12i

| No. | vector             | center                   | mapping |
|-----|--------------------|--------------------------|---------|
| 1   | $[X, Y, Z]$        | $[x, 2x, 0]$             | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[-2x, -x, 0]$           | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[x, -x, 0]$             | [3]     |
| 4   | $[-X, -Y, Z]$      | $[-x, -2x, \frac{1}{2}]$ | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[2x, x, \frac{1}{2}]$   | [5]     |
| 6   | $[X - Y, X, Z]$    | $[-x, x, \frac{1}{2}]$   | [6]     |
| 7   | $[Y, X, -Z]$       | $[2x, x, \frac{1}{2}]$   | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[-x, -2x, \frac{1}{2}]$ | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[-x, x, \frac{1}{2}]$   | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[-2x, -x, 0]$           | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[x, 2x, 0]$             | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[x, -x, 0]$             | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[-x, -2x, 0]$           | [13]    |

*continued ...*

Table 37

| No. | vector             | center                   | mapping |
|-----|--------------------|--------------------------|---------|
| 14  | $[Y, -X + Y, -Z]$  | $[2x, x, 0]$             | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[-x, x, 0]$             | [15]    |
| 16  | $[X, Y, -Z]$       | $[x, 2x, \frac{1}{2}]$   | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[-2x, -x, \frac{1}{2}]$ | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[x, -x, \frac{1}{2}]$   | [18]    |
| 19  | $[-Y, -X, Z]$      | $[-2x, -x, \frac{1}{2}]$ | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[x, 2x, \frac{1}{2}]$   | [20]    |
| 21  | $[X, X - Y, Z]$    | $[x, -x, \frac{1}{2}]$   | [21]    |
| 22  | $[Y, X, Z]$        | $[2x, x, 0]$             | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[-x, -2x, 0]$           | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[-x, x, 0]$             | [24]    |

\* Wyckoff site: 12j, site symmetry: m . .

Table 38: Wyckoff bond: 12a@12j

| No. | vector            | center                      | mapping  |
|-----|-------------------|-----------------------------|----------|
| 1   | $[X, Y, 0]$       | $[x, y, \frac{1}{4}]$       | [1, 16]  |
| 2   | $[-Y, X - Y, 0]$  | $[-y, x - y, \frac{1}{4}]$  | [2, 17]  |
| 3   | $[-X + Y, -X, 0]$ | $[-x + y, -x, \frac{1}{4}]$ | [3, 18]  |
| 4   | $[-X, -Y, 0]$     | $[-x, -y, \frac{3}{4}]$     | [4, 13]  |
| 5   | $[Y, -X + Y, 0]$  | $[y, -x + y, \frac{3}{4}]$  | [5, 14]  |
| 6   | $[X - Y, X, 0]$   | $[x - y, x, \frac{3}{4}]$   | [6, 15]  |
| 7   | $[Y, X, 0]$       | $[y, x, \frac{1}{4}]$       | [7, 22]  |
| 8   | $[X - Y, -Y, 0]$  | $[x - y, -y, \frac{1}{4}]$  | [8, 23]  |
| 9   | $[-X, -X + Y, 0]$ | $[-x, -x + y, \frac{1}{4}]$ | [9, 24]  |
| 10  | $[-Y, -X, 0]$     | $[-y, -x, \frac{3}{4}]$     | [10, 19] |
| 11  | $[-X + Y, Y, 0]$  | $[-x + y, y, \frac{3}{4}]$  | [11, 20] |
| 12  | $[X, X - Y, 0]$   | $[x, x - y, \frac{3}{4}]$   | [12, 21] |

Table 39: Wyckoff bond: 12b@12j

| No. | vector       | center                      | mapping  |
|-----|--------------|-----------------------------|----------|
| 1   | $[0, 0, Z]$  | $[x, y, \frac{1}{4}]$       | [1, -16] |
| 2   | $[0, 0, Z]$  | $[-y, x - y, \frac{1}{4}]$  | [2, -17] |
| 3   | $[0, 0, Z]$  | $[-x + y, -x, \frac{1}{4}]$ | [3, -18] |
| 4   | $[0, 0, Z]$  | $[-x, -y, \frac{3}{4}]$     | [4, -13] |
| 5   | $[0, 0, Z]$  | $[y, -x + y, \frac{3}{4}]$  | [5, -14] |
| 6   | $[0, 0, Z]$  | $[x - y, x, \frac{3}{4}]$   | [6, -15] |
| 7   | $[0, 0, -Z]$ | $[y, x, \frac{1}{4}]$       | [7, -22] |
| 8   | $[0, 0, -Z]$ | $[x - y, -y, \frac{1}{4}]$  | [8, -23] |
| 9   | $[0, 0, -Z]$ | $[-x, -x + y, \frac{1}{4}]$ | [9, -24] |

continued ...

Table 39

| No. | vector       | center                     | mapping  |
|-----|--------------|----------------------------|----------|
| 10  | $[0, 0, -Z]$ | $[-y, -x, \frac{3}{4}]$    | [10,-19] |
| 11  | $[0, 0, -Z]$ | $[-x + y, y, \frac{3}{4}]$ | [11,-20] |
| 12  | $[0, 0, -Z]$ | $[x, x - y, \frac{3}{4}]$  | [12,-21] |

Table 40: Wyckoff bond: 24c@12j

| No. | vector             | center                      | mapping |
|-----|--------------------|-----------------------------|---------|
| 1   | $[X, Y, Z]$        | $[x, y, \frac{1}{4}]$       | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[-y, x - y, \frac{1}{4}]$  | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[-x + y, -x, \frac{1}{4}]$ | [3]     |
| 4   | $[-X, -Y, Z]$      | $[-x, -y, \frac{3}{4}]$     | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[y, -x + y, \frac{3}{4}]$  | [5]     |
| 6   | $[X - Y, X, Z]$    | $[x - y, x, \frac{3}{4}]$   | [6]     |
| 7   | $[Y, X, -Z]$       | $[y, x, \frac{1}{4}]$       | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[x - y, -y, \frac{1}{4}]$  | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[-x, -x + y, \frac{1}{4}]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[-y, -x, \frac{3}{4}]$     | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[-x + y, y, \frac{3}{4}]$  | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[x, x - y, \frac{3}{4}]$   | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[-x, -y, \frac{3}{4}]$     | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[y, -x + y, \frac{3}{4}]$  | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[x - y, x, \frac{3}{4}]$   | [15]    |
| 16  | $[X, Y, -Z]$       | $[x, y, \frac{1}{4}]$       | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[-y, x - y, \frac{1}{4}]$  | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[-x + y, -x, \frac{1}{4}]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[-y, -x, \frac{3}{4}]$     | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[-x + y, y, \frac{3}{4}]$  | [20]    |
| 21  | $[X, X - Y, Z]$    | $[x, x - y, \frac{3}{4}]$   | [21]    |
| 22  | $[Y, X, Z]$        | $[y, x, \frac{1}{4}]$       | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[x - y, -y, \frac{1}{4}]$  | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[-x, -x + y, \frac{1}{4}]$ | [24]    |

\* Wyckoff site: 12k, site symmetry:  $\dots m$

Table 41: Wyckoff bond: 12a@12k

| No. | vector        | center                     | mapping |
|-----|---------------|----------------------------|---------|
| 1   | $[X, 0, Z]$   | $[x, 0, z]$                | [1,23]  |
| 2   | $[0, X, Z]$   | $[0, x, z]$                | [2,22]  |
| 3   | $[-X, -X, Z]$ | $[-x, -x, z]$              | [3,24]  |
| 4   | $[-X, 0, Z]$  | $[-x, 0, z + \frac{1}{2}]$ | [4,20]  |
| 5   | $[0, -X, Z]$  | $[0, -x, z + \frac{1}{2}]$ | [5,19]  |

*continued ...*

Table 41

| No. | vector         | center                      | mapping |
|-----|----------------|-----------------------------|---------|
| 6   | $[X, X, Z]$    | $[x, x, z + \frac{1}{2}]$   | [6,21]  |
| 7   | $[0, X, -Z]$   | $[0, x, \frac{1}{2} - z]$   | [7,17]  |
| 8   | $[X, 0, -Z]$   | $[x, 0, \frac{1}{2} - z]$   | [8,16]  |
| 9   | $[-X, -X, -Z]$ | $[-x, -x, \frac{1}{2} - z]$ | [9,18]  |
| 10  | $[0, -X, -Z]$  | $[0, -x, -z]$               | [10,14] |
| 11  | $[-X, 0, -Z]$  | $[-x, 0, -z]$               | [11,13] |
| 12  | $[X, X, -Z]$   | $[x, x, -z]$                | [12,15] |

Table 42: Wyckoff bond: 12b@12k

| No. | vector         | center                      | mapping  |
|-----|----------------|-----------------------------|----------|
| 1   | $[X, 2X, 0]$   | $[x, 0, z]$                 | [1,-23]  |
| 2   | $[-2X, -X, 0]$ | $[0, x, z]$                 | [2,-22]  |
| 3   | $[X, -X, 0]$   | $[-x, -x, z]$               | [3,-24]  |
| 4   | $[-X, -2X, 0]$ | $[-x, 0, z + \frac{1}{2}]$  | [4,-20]  |
| 5   | $[2X, X, 0]$   | $[0, -x, z + \frac{1}{2}]$  | [5,-19]  |
| 6   | $[-X, X, 0]$   | $[x, x, z + \frac{1}{2}]$   | [6,-21]  |
| 7   | $[2X, X, 0]$   | $[0, x, \frac{1}{2} - z]$   | [7,-17]  |
| 8   | $[-X, -2X, 0]$ | $[x, 0, \frac{1}{2} - z]$   | [8,-16]  |
| 9   | $[-X, X, 0]$   | $[-x, -x, \frac{1}{2} - z]$ | [9,-18]  |
| 10  | $[-2X, -X, 0]$ | $[0, -x, -z]$               | [10,-14] |
| 11  | $[X, 2X, 0]$   | $[-x, 0, -z]$               | [11,-13] |
| 12  | $[X, -X, 0]$   | $[x, x, -z]$                | [12,-15] |

Table 43: Wyckoff bond: 24c@12k

| No. | vector             | center                      | mapping |
|-----|--------------------|-----------------------------|---------|
| 1   | $[X, Y, Z]$        | $[x, 0, z]$                 | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[0, x, z]$                 | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[-x, -x, z]$               | [3]     |
| 4   | $[-X, -Y, Z]$      | $[-x, 0, z + \frac{1}{2}]$  | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[0, -x, z + \frac{1}{2}]$  | [5]     |
| 6   | $[X - Y, X, Z]$    | $[x, x, z + \frac{1}{2}]$   | [6]     |
| 7   | $[Y, X, -Z]$       | $[0, x, \frac{1}{2} - z]$   | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[x, 0, \frac{1}{2} - z]$   | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[-x, -x, \frac{1}{2} - z]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[0, -x, -z]$               | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[-x, 0, -z]$               | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[x, x, -z]$                | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[-x, 0, -z]$               | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[0, -x, -z]$               | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[x, x, -z]$                | [15]    |

continued ...

Table 43

| No. | vector             | center                      | mapping |
|-----|--------------------|-----------------------------|---------|
| 16  | $[X, Y, -Z]$       | $[x, 0, \frac{1}{2} - z]$   | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[0, x, \frac{1}{2} - z]$   | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[-x, -x, \frac{1}{2} - z]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[0, -x, z + \frac{1}{2}]$  | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[-x, 0, z + \frac{1}{2}]$  | [20]    |
| 21  | $[X, X - Y, Z]$    | $[x, x, z + \frac{1}{2}]$   | [21]    |
| 22  | $[Y, X, Z]$        | $[0, x, z]$                 | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[x, 0, z]$                 | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[-x, -x, z]$               | [24]    |

\* Wyckoff site: 241, site symmetry: 1

Table 44: Wyckoff bond: 24a@241

| No. | vector             | center                          | mapping |
|-----|--------------------|---------------------------------|---------|
| 1   | $[X, Y, Z]$        | $[x, y, z]$                     | [1]     |
| 2   | $[-Y, X - Y, Z]$   | $[-y, x - y, z]$                | [2]     |
| 3   | $[-X + Y, -X, Z]$  | $[-x + y, -x, z]$               | [3]     |
| 4   | $[-X, -Y, Z]$      | $[-x, -y, z + \frac{1}{2}]$     | [4]     |
| 5   | $[Y, -X + Y, Z]$   | $[y, -x + y, z + \frac{1}{2}]$  | [5]     |
| 6   | $[X - Y, X, Z]$    | $[x - y, x, z + \frac{1}{2}]$   | [6]     |
| 7   | $[Y, X, -Z]$       | $[y, x, \frac{1}{2} - z]$       | [7]     |
| 8   | $[X - Y, -Y, -Z]$  | $[x - y, -y, \frac{1}{2} - z]$  | [8]     |
| 9   | $[-X, -X + Y, -Z]$ | $[-x, -x + y, \frac{1}{2} - z]$ | [9]     |
| 10  | $[-Y, -X, -Z]$     | $[-y, -x, -z]$                  | [10]    |
| 11  | $[-X + Y, Y, -Z]$  | $[-x + y, y, -z]$               | [11]    |
| 12  | $[X, X - Y, -Z]$   | $[x, x - y, -z]$                | [12]    |
| 13  | $[-X, -Y, -Z]$     | $[-x, -y, -z]$                  | [13]    |
| 14  | $[Y, -X + Y, -Z]$  | $[y, -x + y, -z]$               | [14]    |
| 15  | $[X - Y, X, -Z]$   | $[x - y, x, -z]$                | [15]    |
| 16  | $[X, Y, -Z]$       | $[x, y, \frac{1}{2} - z]$       | [16]    |
| 17  | $[-Y, X - Y, -Z]$  | $[-y, x - y, \frac{1}{2} - z]$  | [17]    |
| 18  | $[-X + Y, -X, -Z]$ | $[-x + y, -x, \frac{1}{2} - z]$ | [18]    |
| 19  | $[-Y, -X, Z]$      | $[-y, -x, z + \frac{1}{2}]$     | [19]    |
| 20  | $[-X + Y, Y, Z]$   | $[-x + y, y, z + \frac{1}{2}]$  | [20]    |
| 21  | $[X, X - Y, Z]$    | $[x, x - y, z + \frac{1}{2}]$   | [21]    |
| 22  | $[Y, X, Z]$        | $[y, x, z]$                     | [22]    |
| 23  | $[X - Y, -Y, Z]$   | $[x - y, -y, z]$                | [23]    |
| 24  | $[-X, -X + Y, Z]$  | $[-x, -x + y, z]$               | [24]    |