

SG No. 125  $D_{4h}^3$   $P4/nbm$  [ tetragonal ]

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

\* Wyckoff site: 2a, site symmetry: 422

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 4b@2a

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

Table 3: Wyckoff bond: 4c@2a

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

Table 4: Wyckoff bond: 8d@2a

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

Table 5: Wyckoff bond: 8e@2a

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

Table 6: Wyckoff bond: 8f@2a

| No. | vector        | center                          | mapping   |
|-----|---------------|---------------------------------|-----------|
| 1   | $[X, Y, 0]$   | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [1, -2]   |
| 2   | $[-Y, X, 0]$  | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [3, -4]   |
| 3   | $[-X, Y, 0]$  | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [5, -6]   |
| 4   | $[Y, X, 0]$   | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [7, -8]   |
| 5   | $[-X, -Y, 0]$ | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [9, -10]  |
| 6   | $[Y, -X, 0]$  | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [11, -12] |
| 7   | $[X, -Y, 0]$  | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [13, -14] |
| 8   | $[-Y, -X, 0]$ | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [15, -16] |

Table 7: Wyckoff bond: 16g@2a

| No. | vector         | center                          | mapping |
|-----|----------------|---------------------------------|---------|
| 1   | $[X, Y, Z]$    | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [1]     |
| 2   | $[-X, -Y, Z]$  | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [2]     |
| 3   | $[-Y, X, Z]$   | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [3]     |
| 4   | $[Y, -X, Z]$   | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [4]     |
| 5   | $[-X, Y, -Z]$  | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [5]     |
| 6   | $[X, -Y, -Z]$  | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [6]     |
| 7   | $[Y, X, -Z]$   | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [7]     |
| 8   | $[-Y, -X, -Z]$ | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [8]     |
| 9   | $[-X, -Y, -Z]$ | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [9]     |
| 10  | $[X, Y, -Z]$   | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [10]    |
| 11  | $[Y, -X, -Z]$  | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [11]    |
| 12  | $[-Y, X, -Z]$  | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [12]    |
| 13  | $[X, -Y, Z]$   | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [13]    |
| 14  | $[-X, Y, Z]$   | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [14]    |
| 15  | $[-Y, -X, Z]$  | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [15]    |
| 16  | $[Y, X, Z]$    | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [16]    |

\* Wyckoff site: 2b, site symmetry: 422

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 4b@2b

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

Table 10: Wyckoff bond: 4c@2b

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

Table 11: Wyckoff bond: 8d@2b

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

Table 12: Wyckoff bond: 8e@2b

| No. | vector       | center                                    | mapping   |
|-----|--------------|---|-----------|
| 1   | [X, X, Z]    | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [1, -8]   |
| 2   | [-X, -X, Z]  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [2, -7]   |
| 3   | [-X, X, Z]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [3, -6]   |
| 4   | [X, -X, Z]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [4, -5]   |
| 5   | [-X, -X, -Z] | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [9, -16]  |
| 6   | [X, X, -Z]   | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [10, -15] |
| 7   | [X, -X, -Z]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [11, -14] |
| 8   | [-X, X, -Z]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [12, -13] |

Table 13: Wyckoff bond: 8f@2b

| No. | vector      | center                                    | mapping   |
|-----|-------------|---|-----------|
| 1   | [X, Y, 0]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [1, -2]   |
| 2   | [-Y, X, 0]  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [3, -4]   |
| 3   | [-X, Y, 0]  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [5, -6]   |
| 4   | [Y, X, 0]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [7, -8]   |
| 5   | [-X, -Y, 0] | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [9, -10]  |
| 6   | [Y, -X, 0]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [11, -12] |
| 7   | [X, -Y, 0]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [13, -14] |
| 8   | [-Y, -X, 0] | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [15, -16] |

Table 14: Wyckoff bond: 16g@2b

| No. | vector       | center                                    | mapping |
|-----|--------------|---|---------|
| 1   | [X, Y, Z]    | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [1]     |
| 2   | [-X, -Y, Z]  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [2]     |
| 3   | [-Y, X, Z]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [3]     |
| 4   | [Y, -X, Z]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [4]     |
| 5   | [-X, Y, -Z]  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [5]     |
| 6   | [X, -Y, -Z]  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [6]     |
| 7   | [Y, X, -Z]   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [7]     |
| 8   | [-Y, -X, -Z] | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [8]     |
| 9   | [-X, -Y, -Z] | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [9]     |
| 10  | [X, Y, -Z]   | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [10]    |
| 11  | [Y, -X, -Z]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [11]    |
| 12  | [-Y, X, -Z]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [12]    |
| 13  | [X, -Y, Z]   | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [13]    |
| 14  | [-X, Y, Z]   | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [14]    |
| 15  | [-Y, -X, Z]  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [15]    |
| 16  | [Y, X, Z]    | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [16]    |

\* Wyckoff site: 2c, site symmetry: -42m

Table 15: Wyckoff bond: 2a@2c

| No. | vector    | center                                     | mapping                          |
|-----|-----------|--|----------------------------------|
| 1   | [0, 0, Z] | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [1, 2, -5, -6, -11, -12, 15, 16] |
| 2   | [0, 0, Z] | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [3, 4, -7, -8, -9, -10, 13, 14]  |

Table 16: Wyckoff bond: 4b@2c

| No. | vector     | center                                     | mapping            |
|-----|------------|--|--------------------|
| 1   | [X, 0, 0]  | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [1, -2, -5, 6]     |
| 2   | [0, X, 0]  | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [3, -4, 7, -8]     |
| 3   | [-X, 0, 0] | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [9, -10, -13, 14]  |
| 4   | [0, -X, 0] | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [11, -12, 15, -16] |

Table 17: Wyckoff bond: 4c@2c

| No. | vector     | center                                     | mapping          |
|-----|------------|--|------------------|
| 1   | [X, X, 0]  | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [1, -2, -15, 16] |
| 2   | [-X, X, 0] | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [3, -4, -13, 14] |
| 3   | [-X, X, 0] | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [5, -6, -11, 12] |
| 4   | [X, X, 0]  | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [7, -8, -9, 10]  |

Table 18: Wyckoff bond: 8d@2c

| No. | vector      | center                                     | mapping   |
|-----|-------------|--|-----------|
| 1   | [X, 0, Z]   | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [1, -5]   |
| 2   | [-X, 0, Z]  | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [2, -6]   |
| 3   | [0, X, Z]   | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [3, -8]   |
| 4   | [0, -X, Z]  | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [4, -7]   |
| 5   | [-X, 0, -Z] | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [9, -13]  |
| 6   | [X, 0, -Z]  | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [10, -14] |
| 7   | [0, -X, -Z] | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [11, -16] |
| 8   | [0, X, -Z]  | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [12, -15] |

Table 19: Wyckoff bond: 8e@2c

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

Table 20: Wyckoff bond: 8f@2c

| No. | vector        | center                          | mapping   |
|-----|---------------|---------------------------------|-----------|
| 1   | $[X, Y, 0]$   | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [1, -2]   |
| 2   | $[-Y, X, 0]$  | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [3, -4]   |
| 3   | $[-X, Y, 0]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [5, -6]   |
| 4   | $[Y, X, 0]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [7, -8]   |
| 5   | $[-X, -Y, 0]$ | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [9, -10]  |
| 6   | $[Y, -X, 0]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [11, -12] |
| 7   | $[X, -Y, 0]$  | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [13, -14] |
| 8   | $[-Y, -X, 0]$ | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [15, -16] |

Table 21: Wyckoff bond: 16g@2c

| No. | vector         | center                          | mapping |
|-----|----------------|---------------------------------|---------|
| 1   | $[X, Y, Z]$    | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [1]     |
| 2   | $[-X, -Y, Z]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [2]     |
| 3   | $[-Y, X, Z]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [3]     |
| 4   | $[Y, -X, Z]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [4]     |
| 5   | $[-X, Y, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [5]     |
| 6   | $[X, -Y, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [6]     |
| 7   | $[Y, X, -Z]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [7]     |
| 8   | $[-Y, -X, -Z]$ | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [8]     |
| 9   | $[-X, -Y, -Z]$ | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [9]     |
| 10  | $[X, Y, -Z]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [10]    |
| 11  | $[Y, -X, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [11]    |
| 12  | $[-Y, X, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [12]    |
| 13  | $[X, -Y, Z]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [13]    |
| 14  | $[-X, Y, Z]$   | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [14]    |
| 15  | $[-Y, -X, Z]$  | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [15]    |
| 16  | $[Y, X, Z]$    | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [16]    |

\* Wyckoff site: 2d, site symmetry: -42m

Table 22: Wyckoff bond: 2a@2d

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

Table 23: Wyckoff bond: 4b@2d

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

Table 24: Wyckoff bond: 4c@2d

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

Table 25: Wyckoff bond: 8d@2d

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

Table 26: Wyckoff bond: 8e@2d

| No. | vector       | center  | mapping |
|-----|--------------|---|---------|
| 1   | [X, X, Z]    | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [1, 16] |
| 2   | [-X, -X, Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [2, 15] |
| 3   | [-X, X, Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [3, 14] |
| 4   | [X, -X, Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [4, 13] |
| 5   | [-X, X, -Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [5, 12] |
| 6   | [X, -X, -Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [6, 11] |
| 7   | [X, X, -Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [7, 10] |
| 8   | [-X, -X, -Z] | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [8, 9]  |

Table 27: Wyckoff bond: 8f@2d

| No. | vector      | center  | mapping   |
|-----|-------------|---|-----------|
| 1   | [X, Y, 0]   | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [1, -2]   |
| 2   | [-Y, X, 0]  | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [3, -4]   |
| 3   | [-X, Y, 0]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [5, -6]   |
| 4   | [Y, X, 0]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [7, -8]   |
| 5   | [-X, -Y, 0] | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [9, -10]  |
| 6   | [Y, -X, 0]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [11, -12] |
| 7   | [X, -Y, 0]  | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [13, -14] |
| 8   | [-Y, -X, 0] | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [15, -16] |

Table 28: Wyckoff bond: 16g@2d

| No. | vector       | center  | mapping |
|-----|--------------|---|---------|
| 1   | [X, Y, Z]    | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [1]     |
| 2   | [-X, -Y, Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [2]     |
| 3   | [-Y, X, Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [3]     |
| 4   | [Y, -X, Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [4]     |
| 5   | [-X, Y, -Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [5]     |
| 6   | [X, -Y, -Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [6]     |
| 7   | [Y, X, -Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [7]     |
| 8   | [-Y, -X, -Z] | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [8]     |
| 9   | [-X, -Y, -Z] | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [9]     |
| 10  | [X, Y, -Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [10]    |
| 11  | [Y, -X, -Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [11]    |
| 12  | [-Y, X, -Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [12]    |
| 13  | [X, -Y, Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [13]    |
| 14  | [-X, Y, Z]   | [ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ] | [14]    |
| 15  | [-Y, -X, Z]  | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [15]    |
| 16  | [Y, X, Z]    | [ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{2}$ ] | [16]    |

\* Wyckoff site: **4e**, site symmetry:  $\dots 2/m$

Table 29: Wyckoff bond: **4a@4e**

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

Table 30: Wyckoff bond: **4b@4e**

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

Table 31: Wyckoff bond: **8c@4e**

| No. | vector         | center                          | mapping    |
|-----|----------------|---------------------------------|------------|
| 1   | $[X, Y, Z]$    | $[0, 0, 0]$                     | $[1, -9]$  |
| 2   | $[-X, -Y, Z]$  | $[\frac{1}{2}, \frac{1}{2}, 0]$ | $[2, -10]$ |
| 3   | $[-Y, X, Z]$   | $[\frac{1}{2}, 0, 0]$           | $[3, -11]$ |
| 4   | $[Y, -X, Z]$   | $[0, \frac{1}{2}, 0]$           | $[4, -12]$ |
| 5   | $[-X, Y, -Z]$  | $[\frac{1}{2}, 0, 0]$           | $[5, -13]$ |
| 6   | $[X, -Y, -Z]$  | $[0, \frac{1}{2}, 0]$           | $[6, -14]$ |
| 7   | $[Y, X, -Z]$   | $[0, 0, 0]$                     | $[7, -15]$ |
| 8   | $[-Y, -X, -Z]$ | $[\frac{1}{2}, \frac{1}{2}, 0]$ | $[8, -16]$ |

\* Wyckoff site: **4f**, site symmetry:  $\dots 2/m$

Table 32: Wyckoff bond: **4a@4f**

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

Table 33: Wyckoff bond: 4b@4f

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

Table 34: Wyckoff bond: 8c@4f

| No. | vector         | center                                    | mapping    |
|-----|----------------|---|------------|
| 1   | $[X, Y, Z]$    | $[0, 0, \frac{1}{2}]$                     | $[1, -9]$  |
| 2   | $[-X, -Y, Z]$  | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[2, -10]$ |
| 3   | $[-Y, X, Z]$   | $[\frac{1}{2}, 0, \frac{1}{2}]$           | $[3, -11]$ |
| 4   | $[Y, -X, Z]$   | $[0, \frac{1}{2}, \frac{1}{2}]$           | $[4, -12]$ |
| 5   | $[-X, Y, -Z]$  | $[\frac{1}{2}, 0, \frac{1}{2}]$           | $[5, -13]$ |
| 6   | $[X, -Y, -Z]$  | $[0, \frac{1}{2}, \frac{1}{2}]$           | $[6, -14]$ |
| 7   | $[Y, X, -Z]$   | $[0, 0, \frac{1}{2}]$                     | $[7, -15]$ |
| 8   | $[-Y, -X, -Z]$ | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[8, -16]$ |

\* Wyckoff site: 4g, site symmetry: 4..

Table 35: Wyckoff bond: 4a@4g

| No. | vector       | center                           | mapping            |
|-----|--------------|----------------------------------|--------------------|
| 1   | $[0, 0, Z]$  | $[\frac{1}{4}, \frac{1}{4}, z]$  | $[1, 2, 3, 4]$     |
| 2   | $[0, 0, -Z]$ | $[\frac{1}{4}, \frac{1}{4}, -z]$ | $[5, 6, 7, 8]$     |
| 3   | $[0, 0, -Z]$ | $[\frac{3}{4}, \frac{3}{4}, -z]$ | $[9, 10, 11, 12]$  |
| 4   | $[0, 0, Z]$  | $[\frac{3}{4}, \frac{3}{4}, z]$  | $[13, 14, 15, 16]$ |

Table 36: Wyckoff bond: 8b@4g

| No. | vector        | center                           | mapping     |
|-----|---------------|----------------------------------|-------------|
| 1   | $[X, Y, 0]$   | $[\frac{1}{4}, \frac{1}{4}, z]$  | $[1, -2]$   |
| 2   | $[-Y, X, 0]$  | $[\frac{1}{4}, \frac{1}{4}, z]$  | $[3, -4]$   |
| 3   | $[-X, Y, 0]$  | $[\frac{1}{4}, \frac{1}{4}, -z]$ | $[5, -6]$   |
| 4   | $[Y, X, 0]$   | $[\frac{1}{4}, \frac{1}{4}, -z]$ | $[7, -8]$   |
| 5   | $[-X, -Y, 0]$ | $[\frac{3}{4}, \frac{3}{4}, -z]$ | $[9, -10]$  |
| 6   | $[Y, -X, 0]$  | $[\frac{3}{4}, \frac{3}{4}, -z]$ | $[11, -12]$ |
| 7   | $[X, -Y, 0]$  | $[\frac{3}{4}, \frac{3}{4}, z]$  | $[13, -14]$ |
| 8   | $[-Y, -X, 0]$ | $[\frac{3}{4}, \frac{3}{4}, z]$  | $[15, -16]$ |

Table 37: Wyckoff bond: 16c@4g

| No. | vector         | center                           | mapping |
|-----|----------------|----------------------------------|---------|
| 1   | $[X, Y, Z]$    | $[\frac{1}{4}, \frac{1}{4}, z]$  | [1]     |
| 2   | $[-X, -Y, Z]$  | $[\frac{1}{4}, \frac{1}{4}, z]$  | [2]     |
| 3   | $[-Y, X, Z]$   | $[\frac{1}{4}, \frac{1}{4}, z]$  | [3]     |
| 4   | $[Y, -X, Z]$   | $[\frac{1}{4}, \frac{1}{4}, z]$  | [4]     |
| 5   | $[-X, Y, -Z]$  | $[\frac{1}{4}, \frac{1}{4}, -z]$ | [5]     |
| 6   | $[X, -Y, -Z]$  | $[\frac{1}{4}, \frac{1}{4}, -z]$ | [6]     |
| 7   | $[Y, X, -Z]$   | $[\frac{1}{4}, \frac{1}{4}, -z]$ | [7]     |
| 8   | $[-Y, -X, -Z]$ | $[\frac{1}{4}, \frac{1}{4}, -z]$ | [8]     |
| 9   | $[-X, -Y, -Z]$ | $[\frac{3}{4}, \frac{3}{4}, -z]$ | [9]     |
| 10  | $[X, Y, -Z]$   | $[\frac{3}{4}, \frac{3}{4}, -z]$ | [10]    |
| 11  | $[Y, -X, -Z]$  | $[\frac{3}{4}, \frac{3}{4}, -z]$ | [11]    |
| 12  | $[-Y, X, -Z]$  | $[\frac{3}{4}, \frac{3}{4}, -z]$ | [12]    |
| 13  | $[X, -Y, Z]$   | $[\frac{3}{4}, \frac{3}{4}, z]$  | [13]    |
| 14  | $[-X, Y, Z]$   | $[\frac{3}{4}, \frac{3}{4}, z]$  | [14]    |
| 15  | $[-Y, -X, Z]$  | $[\frac{3}{4}, \frac{3}{4}, z]$  | [15]    |
| 16  | $[Y, X, Z]$    | $[\frac{3}{4}, \frac{3}{4}, z]$  | [16]    |

\* Wyckoff site: 4h, site symmetry: 2..mm

Table 38: Wyckoff bond: 4a@4h

| No. | vector       | center                           | mapping          |
|-----|--------------|----------------------------------|------------------|
| 1   | $[X, X, 0]$  | $[\frac{3}{4}, \frac{1}{4}, z]$  | [1, -2, -15, 16] |
| 2   | $[-X, X, 0]$ | $[\frac{1}{4}, \frac{3}{4}, z]$  | [3, -4, -13, 14] |
| 3   | $[-X, X, 0]$ | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [5, -6, -11, 12] |
| 4   | $[X, X, 0]$  | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [7, -8, -9, 10]  |

Table 39: Wyckoff bond: 4b@4h

| No. | vector       | center                           | mapping        |
|-----|--------------|----------------------------------|----------------|
| 1   | $[0, 0, Z]$  | $[\frac{3}{4}, \frac{1}{4}, z]$  | [1, 2, 15, 16] |
| 2   | $[0, 0, Z]$  | $[\frac{1}{4}, \frac{3}{4}, z]$  | [3, 4, 13, 14] |
| 3   | $[0, 0, -Z]$ | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [5, 6, 11, 12] |
| 4   | $[0, 0, -Z]$ | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [7, 8, 9, 10]  |

Table 40: Wyckoff bond: 8c@4h

| No. | vector      | center                          | mapping |
|-----|-------------|---------------------------------|---------|
| 1   | $[X, X, Z]$ | $[\frac{3}{4}, \frac{1}{4}, z]$ | [1, 16] |

*continued ...*

Table 40

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

Table 41: Wyckoff bond: 8d@4h

| No. | vector        | center                           | mapping  |
|-----|---------------|----------------------------------|----------|
| 1   | $[X, Y, 0]$   | $[\frac{3}{4}, \frac{1}{4}, z]$  | [1,-2]   |
| 2   | $[-Y, X, 0]$  | $[\frac{1}{4}, \frac{3}{4}, z]$  | [3,-4]   |
| 3   | $[-X, Y, 0]$  | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [5,-6]   |
| 4   | $[Y, X, 0]$   | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [7,-8]   |
| 5   | $[-X, -Y, 0]$ | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [9,-10]  |
| 6   | $[Y, -X, 0]$  | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [11,-12] |
| 7   | $[X, -Y, 0]$  | $[\frac{1}{4}, \frac{3}{4}, z]$  | [13,-14] |
| 8   | $[-Y, -X, 0]$ | $[\frac{3}{4}, \frac{1}{4}, z]$  | [15,-16] |

Table 42: Wyckoff bond: 16e@4h

| No. | vector         | center                           | mapping |
|-----|----------------|----------------------------------|---------|
| 1   | $[X, Y, Z]$    | $[\frac{3}{4}, \frac{1}{4}, z]$  | [1]     |
| 2   | $[-X, -Y, Z]$  | $[\frac{3}{4}, \frac{1}{4}, z]$  | [2]     |
| 3   | $[-Y, X, Z]$   | $[\frac{1}{4}, \frac{3}{4}, z]$  | [3]     |
| 4   | $[Y, -X, Z]$   | $[\frac{1}{4}, \frac{3}{4}, z]$  | [4]     |
| 5   | $[-X, Y, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [5]     |
| 6   | $[X, -Y, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [6]     |
| 7   | $[Y, X, -Z]$   | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [7]     |
| 8   | $[-Y, -X, -Z]$ | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [8]     |
| 9   | $[-X, -Y, -Z]$ | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [9]     |
| 10  | $[X, Y, -Z]$   | $[\frac{1}{4}, \frac{3}{4}, -z]$ | [10]    |
| 11  | $[Y, -X, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [11]    |
| 12  | $[-Y, X, -Z]$  | $[\frac{3}{4}, \frac{1}{4}, -z]$ | [12]    |
| 13  | $[X, -Y, Z]$   | $[\frac{1}{4}, \frac{3}{4}, z]$  | [13]    |
| 14  | $[-X, Y, Z]$   | $[\frac{1}{4}, \frac{3}{4}, z]$  | [14]    |
| 15  | $[-Y, -X, Z]$  | $[\frac{3}{4}, \frac{1}{4}, z]$  | [15]    |
| 16  | $[Y, X, Z]$    | $[\frac{3}{4}, \frac{1}{4}, z]$  | [16]    |

\* Wyckoff site: 8i, site symmetry: ...2

Table 43: Wyckoff bond: 8a@8i

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

Table 44: Wyckoff bond: 8b@8i

| No. | vector        | center                                  | mapping |
|-----|---------------|---|---------|
| 1   | $[X, X, 0]$   | $[x, x, 0]$                             | [1,7]   |
| 2   | $[-X, -X, 0]$ | $[\frac{1}{2} - x, \frac{1}{2} - x, 0]$ | [2,8]   |
| 3   | $[-X, X, 0]$  | $[\frac{1}{2} - x, x, 0]$               | [3,5]   |
| 4   | $[X, -X, 0]$  | $[x, \frac{1}{2} - x, 0]$               | [4,6]   |
| 5   | $[-X, -X, 0]$ | $[-x, -x, 0]$                           | [9,15]  |
| 6   | $[X, X, 0]$   | $[x + \frac{1}{2}, x + \frac{1}{2}, 0]$ | [10,16] |
| 7   | $[X, -X, 0]$  | $[x + \frac{1}{2}, -x, 0]$              | [11,13] |
| 8   | $[-X, X, 0]$  | $[-x, x + \frac{1}{2}, 0]$              | [12,14] |

Table 45: Wyckoff bond: 16c@8i

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

\* Wyckoff site: 8j, site symmetry: . . 2

Table 46: Wyckoff bond: 8a@8j

| No. | vector         | center  | mapping   |
|-----|----------------|---|-----------|
| 1   | $[X, -X, Z]$   | $[x, x, \frac{1}{2}]$                             | [1, -7]   |
| 2   | $[-X, X, Z]$   | $[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$ | [2, -8]   |
| 3   | $[X, X, Z]$    | $[\frac{1}{2} - x, x, \frac{1}{2}]$               | [3, -5]   |
| 4   | $[-X, -X, Z]$  | $[x, \frac{1}{2} - x, \frac{1}{2}]$               | [4, -6]   |
| 5   | $[-X, X, -Z]$  | $[-x, -x, \frac{1}{2}]$                           | [9, -15]  |
| 6   | $[X, -X, -Z]$  | $[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$ | [10, -16] |
| 7   | $[-X, -X, -Z]$ | $[x + \frac{1}{2}, -x, \frac{1}{2}]$              | [11, -13] |
| 8   | $[X, X, -Z]$   | $[-x, x + \frac{1}{2}, \frac{1}{2}]$              | [12, -14] |

Table 47: Wyckoff bond: 8b@8j

| No. | vector        | center  | mapping  |
|-----|---------------|---|----------|
| 1   | $[X, X, 0]$   | $[x, x, \frac{1}{2}]$                             | [1, 7]   |
| 2   | $[-X, -X, 0]$ | $[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$ | [2, 8]   |
| 3   | $[-X, X, 0]$  | $[\frac{1}{2} - x, x, \frac{1}{2}]$               | [3, 5]   |
| 4   | $[X, -X, 0]$  | $[x, \frac{1}{2} - x, \frac{1}{2}]$               | [4, 6]   |
| 5   | $[-X, -X, 0]$ | $[-x, -x, \frac{1}{2}]$                           | [9, 15]  |
| 6   | $[X, X, 0]$   | $[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$ | [10, 16] |
| 7   | $[X, -X, 0]$  | $[x + \frac{1}{2}, -x, \frac{1}{2}]$              | [11, 13] |
| 8   | $[-X, X, 0]$  | $[-x, x + \frac{1}{2}, \frac{1}{2}]$              | [12, 14] |

Table 48: Wyckoff bond: 16c@8j

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

*continued ...*

Table 48

| No. | vector      | center  | mapping |
|-----|-------------|---|---------|
| 16  | $[Y, X, Z]$ | $[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$ | [16]    |

\* Wyckoff site: 8k, site symmetry: .2.

Table 49: Wyckoff bond: 8a@8k

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

Table 50: Wyckoff bond: 8b@8k

| No. | vector       | center                              | mapping |
|-----|--------------|-------------------------------------|---------|
| 1   | $[X, 0, 0]$  | $[x, \frac{1}{4}, 0]$               | [1,6]   |
| 2   | $[-X, 0, 0]$ | $[\frac{1}{2} - x, \frac{1}{4}, 0]$ | [2,5]   |
| 3   | $[0, X, 0]$  | $[\frac{1}{4}, x, 0]$               | [3,7]   |
| 4   | $[0, -X, 0]$ | $[\frac{1}{4}, \frac{1}{2} - x, 0]$ | [4,8]   |
| 5   | $[-X, 0, 0]$ | $[-x, \frac{3}{4}, 0]$              | [9,14]  |
| 6   | $[X, 0, 0]$  | $[x + \frac{1}{2}, \frac{3}{4}, 0]$ | [10,13] |
| 7   | $[0, -X, 0]$ | $[\frac{3}{4}, -x, 0]$              | [11,15] |
| 8   | $[0, X, 0]$  | $[\frac{3}{4}, x + \frac{1}{2}, 0]$ | [12,16] |

Table 51: Wyckoff bond: 16c@8k

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

*continued ...*

Table 51

| No. | vector        | center                              | mapping |
|-----|---------------|-------------------------------------|---------|
| 10  | $[X, Y, -Z]$  | $[x + \frac{1}{2}, \frac{3}{4}, 0]$ | [10]    |
| 11  | $[Y, -X, -Z]$ | $[\frac{3}{4}, -x, 0]$              | [11]    |
| 12  | $[-Y, X, -Z]$ | $[\frac{3}{4}, x + \frac{1}{2}, 0]$ | [12]    |
| 13  | $[X, -Y, Z]$  | $[x + \frac{1}{2}, \frac{3}{4}, 0]$ | [13]    |
| 14  | $[-X, Y, Z]$  | $[-x, \frac{3}{4}, 0]$              | [14]    |
| 15  | $[-Y, -X, Z]$ | $[\frac{3}{4}, -x, 0]$              | [15]    |
| 16  | $[Y, X, Z]$   | $[\frac{3}{4}, x + \frac{1}{2}, 0]$ | [16]    |

\* Wyckoff site: 81, site symmetry: .2.

Table 52: Wyckoff bond: 8a@81

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

Table 53: Wyckoff bond: 8b@81

| No. | vector       | center  | mapping |
|-----|--------------|---|---------|
| 1   | $[X, 0, 0]$  | $[x, \frac{1}{4}, \frac{1}{2}]$               | [1,6]   |
| 2   | $[-X, 0, 0]$ | $[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2}]$ | [2,5]   |
| 3   | $[0, X, 0]$  | $[\frac{1}{4}, x, \frac{1}{2}]$               | [3,7]   |
| 4   | $[0, -X, 0]$ | $[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}]$ | [4,8]   |
| 5   | $[-X, 0, 0]$ | $[-x, \frac{3}{4}, \frac{1}{2}]$              | [9,14]  |
| 6   | $[X, 0, 0]$  | $[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$ | [10,13] |
| 7   | $[0, -X, 0]$ | $[\frac{3}{4}, -x, \frac{1}{2}]$              | [11,15] |
| 8   | $[0, X, 0]$  | $[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}]$ | [12,16] |

Table 54: Wyckoff bond: 16c@81

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

*continued ...*

Table 54

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

\* Wyckoff site: 8m, site symmetry: . . m

Table 55: Wyckoff bond: 8a@8m

| No. | vector         | center                                   | mapping |
|-----|----------------|--|---------|
| 1   | $[X, -X, Z]$   | $[x, -x, z]$                             | [1, 15] |
| 2   | $[-X, X, Z]$   | $[\frac{1}{2} - x, x + \frac{1}{2}, z]$  | [2, 16] |
| 3   | $[X, X, Z]$    | $[x + \frac{1}{2}, x, z]$                | [3, 13] |
| 4   | $[-X, -X, Z]$  | $[-x, \frac{1}{2} - x, z]$               | [4, 14] |
| 5   | $[-X, -X, -Z]$ | $[\frac{1}{2} - x, -x, -z]$              | [5, 11] |
| 6   | $[X, X, -Z]$   | $[x, x + \frac{1}{2}, -z]$               | [6, 12] |
| 7   | $[-X, X, -Z]$  | $[-x, x, -z]$                            | [7, 9]  |
| 8   | $[X, -X, -Z]$  | $[x + \frac{1}{2}, \frac{1}{2} - x, -z]$ | [8, 10] |

Table 56: Wyckoff bond: 8b@8m

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

Table 57: Wyckoff bond: 16c@8m

| No. | vector       | center                                 | mapping |
|-----|--------------|--|---------|
| 1   | [X, Y, Z]    | [x, -x, z]                             | [1]     |
| 2   | [-X, -Y, Z]  | [\frac{1}{2} - x, x + \frac{1}{2}, z]  | [2]     |
| 3   | [-Y, X, Z]   | [x + \frac{1}{2}, x, z]                | [3]     |
| 4   | [Y, -X, Z]   | [-x, \frac{1}{2} - x, z]               | [4]     |
| 5   | [-X, Y, -Z]  | [\frac{1}{2} - x, -x, -z]              | [5]     |
| 6   | [X, -Y, -Z]  | [x, x + \frac{1}{2}, -z]               | [6]     |
| 7   | [Y, X, -Z]   | [-x, x, -z]                            | [7]     |
| 8   | [-Y, -X, -Z] | [x + \frac{1}{2}, \frac{1}{2} - x, -z] | [8]     |
| 9   | [-X, -Y, -Z] | [-x, x, -z]                            | [9]     |
| 10  | [X, Y, -Z]   | [x + \frac{1}{2}, \frac{1}{2} - x, -z] | [10]    |
| 11  | [Y, -X, -Z]  | [\frac{1}{2} - x, -x, -z]              | [11]    |
| 12  | [-Y, X, -Z]  | [x, x + \frac{1}{2}, -z]               | [12]    |
| 13  | [X, -Y, Z]   | [x + \frac{1}{2}, x, z]                | [13]    |
| 14  | [-X, Y, Z]   | [-x, \frac{1}{2} - x, z]               | [14]    |
| 15  | [-Y, -X, Z]  | [x, -x, z]                             | [15]    |
| 16  | [Y, X, Z]    | [\frac{1}{2} - x, x + \frac{1}{2}, z]  | [16]    |

\* Wyckoff site: 16n, site symmetry: 1

Table 58: Wyckoff bond: 16a@16n

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