

* Wyckoff site: 2a, site symmetry: $6..$

Table 1: Wyckoff bond: 2a@2a

| No. | vector | center | mapping |
|-----|--------------|--------------|-------------------------|
| 1 | $[0, 0, Z]$ | $[0, 0, z]$ | $[1, 2, 3, 4, 5, 6]$ |
| 2 | $[0, 0, -Z]$ | $[0, 0, -z]$ | $[7, 8, 9, 10, 11, 12]$ |

Table 2: Wyckoff bond: 6b@2a

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

Table 3: Wyckoff bond: 12c@2a

| 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 | $[-X, -Y, Z]$ | $[0, 0, z]$ | $[4]$ |
| 5 | $[Y, -X + Y, Z]$ | $[0, 0, z]$ | $[5]$ |
| 6 | $[X - Y, X, Z]$ | $[0, 0, z]$ | $[6]$ |
| 7 | $[Y, X, -Z]$ | $[0, 0, -z]$ | $[7]$ |
| 8 | $[X - Y, -Y, -Z]$ | $[0, 0, -z]$ | $[8]$ |
| 9 | $[-X, -X + Y, -Z]$ | $[0, 0, -z]$ | $[9]$ |
| 10 | $[-Y, -X, -Z]$ | $[0, 0, -z]$ | $[10]$ |
| 11 | $[-X + Y, Y, -Z]$ | $[0, 0, -z]$ | $[11]$ |
| 12 | $[X, X - Y, -Z]$ | $[0, 0, -z]$ | $[12]$ |

 * Wyckoff site: 6b, site symmetry: $.2.$

Table 4: Wyckoff bond: 6a@6b

| No. | vector | center | mapping |
|-----|----------------|-------------|-----------|
| 1 | $[X, 2X, Z]$ | $[x, 0, 0]$ | $[1, -8]$ |
| 2 | $[-2X, -X, Z]$ | $[0, x, 0]$ | $[2, -7]$ |

continued ...

Table 4

| No. | vector | center | mapping |
|-----|----------------|---------------|------------|
| 3 | $[X, -X, Z]$ | $[-x, -x, 0]$ | $[3, -9]$ |
| 4 | $[-X, -2X, Z]$ | $[-x, 0, 0]$ | $[4, -11]$ |
| 5 | $[2X, X, Z]$ | $[0, -x, 0]$ | $[5, -10]$ |
| 6 | $[-X, X, Z]$ | $[x, x, 0]$ | $[6, -12]$ |

Table 5: Wyckoff bond: **6b@6b**

| No. | vector | center | mapping |
|-----|---------------|---------------|-----------|
| 1 | $[X, 0, 0]$ | $[x, 0, 0]$ | $[1, 8]$ |
| 2 | $[0, X, 0]$ | $[0, x, 0]$ | $[2, 7]$ |
| 3 | $[-X, -X, 0]$ | $[-x, -x, 0]$ | $[3, 9]$ |
| 4 | $[-X, 0, 0]$ | $[-x, 0, 0]$ | $[4, 11]$ |
| 5 | $[0, -X, 0]$ | $[0, -x, 0]$ | $[5, 10]$ |
| 6 | $[X, X, 0]$ | $[x, x, 0]$ | $[6, 12]$ |

Table 6: Wyckoff bond: **12c@6b**

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

* Wyckoff site: **6c**, site symmetry: $\dots 2$

Table 7: Wyckoff bond: **6a@6c**

| No. | vector | center | mapping |
|-----|---------------|----------------|------------|
| 1 | $[X, X, Z]$ | $[x, -x, 0]$ | $[1, -10]$ |
| 2 | $[-X, 0, Z]$ | $[x, 2x, 0]$ | $[2, -12]$ |
| 3 | $[0, -X, Z]$ | $[-2x, -x, 0]$ | $[3, -11]$ |
| 4 | $[-X, -X, Z]$ | $[-x, x, 0]$ | $[4, -7]$ |

continued ...

Table 7

| No. | vector | center | mapping |
|-----|-------------|----------------|-----------|
| 5 | $[X, 0, Z]$ | $[-x, -2x, 0]$ | $[5, -9]$ |
| 6 | $[0, X, Z]$ | $[2x, x, 0]$ | $[6, -8]$ |

Table 8: Wyckoff bond: **6b@6c**

| No. | vector | center | mapping |
|-----|----------------|----------------|-----------|
| 1 | $[X, -X, 0]$ | $[x, -x, 0]$ | $[1, 10]$ |
| 2 | $[X, 2X, 0]$ | $[x, 2x, 0]$ | $[2, 12]$ |
| 3 | $[-2X, -X, 0]$ | $[-2x, -x, 0]$ | $[3, 11]$ |
| 4 | $[-X, X, 0]$ | $[-x, x, 0]$ | $[4, 7]$ |
| 5 | $[-X, -2X, 0]$ | $[-x, -2x, 0]$ | $[5, 9]$ |
| 6 | $[2X, X, 0]$ | $[2x, x, 0]$ | $[6, 8]$ |

Table 9: Wyckoff bond: **12c@6c**

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

* Wyckoff site: 12d, site symmetry: 1

Table 10: Wyckoff bond: **12a@12d**

| 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 | $[-X, -Y, Z]$ | $[-x, -y, z]$ | $[4]$ |
| 5 | $[Y, -X + Y, Z]$ | $[y, -x + y, z]$ | $[5]$ |
| 6 | $[X - Y, X, Z]$ | $[x - y, x, z]$ | $[6]$ |

continued ...

Table 10

| No. | vector | center | mapping |
|-----|--------------------|--------------------|---------|
| 7 | $[Y, X, -Z]$ | $[y, x, -z]$ | [7] |
| 8 | $[X - Y, -Y, -Z]$ | $[x - y, -y, -z]$ | [8] |
| 9 | $[-X, -X + Y, -Z]$ | $[-x, -x + y, -z]$ | [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] |