

SG No. 10  $C_{2h}^1$   $P2/m$  (b-axis setting) [ monoclinic ]

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

\* Wyckoff site: 1a, site symmetry: 2/m

Table 1: Wyckoff bond: 1a@1a

No.	vector	center	mapping
1	[X, 0, Z]	[0, 0, 0]	[1, -2, -3, 4]

Table 2: Wyckoff bond: 1b@1a

No.	vector	center	mapping
1	[0, Y, 0]	[0, 0, 0]	[1, 2, -3, -4]

Table 3: Wyckoff bond: 2c@1a

No.	vector	center	mapping
1	[X, Y, Z]	[0, 0, 0]	[1, -3]
2	[-X, Y, -Z]	[0, 0, 0]	[2, -4]

\* Wyckoff site: 1b, site symmetry: 2/m

Table 4: Wyckoff bond: 1a@1b

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

Table 5: Wyckoff bond: 1b@1b

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

Table 6: Wyckoff bond: 2c@1b

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

\* Wyckoff site: **1c**, site symmetry:  $2/m$

Table 7: Wyckoff bond: **1a@1c**

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

Table 8: Wyckoff bond: **1b@1c**

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

Table 9: Wyckoff bond: **2c@1c**

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

\* Wyckoff site: **1d**, site symmetry:  $2/m$

Table 10: Wyckoff bond: **1a@1d**

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

Table 11: Wyckoff bond: **1b@1d**

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

Table 12: Wyckoff bond: **2c@1d**

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

\* Wyckoff site: **1e**, site symmetry:  $2/m$

Table 13: Wyckoff bond: **1a@1e**

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

Table 14: Wyckoff bond: **1b@1e**

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

Table 15: Wyckoff bond: **2c@1e**

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

\* Wyckoff site: **1f**, site symmetry:  $2/m$

Table 16: Wyckoff bond: **1a@1f**

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

Table 17: Wyckoff bond: **1b@1f**

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

Table 18: Wyckoff bond: **2c@1f**

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

\* Wyckoff site: **1g**, site symmetry:  $2/m$

Table 19: Wyckoff bond: **1a@1g**

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

Table 20: Wyckoff bond: **1b@1g**

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

Table 21: Wyckoff bond: **2c@1g**

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

\* Wyckoff site: **1h**, site symmetry:  $2/m$

Table 22: Wyckoff bond: **1a@1h**

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

Table 23: Wyckoff bond: **1b@1h**

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

Table 24: Wyckoff bond: **2c@1h**

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

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

Table 25: Wyckoff bond: 2a@2i

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, 0]$	$[1, -2]$
2	$[-X, 0, -Z]$	$[0, -y, 0]$	$[3, -4]$

Table 26: Wyckoff bond: 2b@2i

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, 0]$	$[1, 2]$
2	$[0, -Y, 0]$	$[0, -y, 0]$	$[3, 4]$

Table 27: Wyckoff bond: 4c@2i

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, 0]$	$[1]$
2	$[-X, Y, -Z]$	$[0, y, 0]$	$[2]$
3	$[-X, -Y, -Z]$	$[0, -y, 0]$	$[3]$
4	$[X, -Y, Z]$	$[0, -y, 0]$	$[4]$

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

Table 28: Wyckoff bond: 2a@2j

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, y, 0]$	$[1, -2]$
2	$[-X, 0, -Z]$	$[\frac{1}{2}, -y, 0]$	$[3, -4]$

Table 29: Wyckoff bond: 2b@2j

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

Table 30: Wyckoff bond: 4c@2j

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

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

Table 31: Wyckoff bond: 2a@2k

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, \frac{1}{2}]$	[1, -2]
2	$[-X, 0, -Z]$	$[0, -y, \frac{1}{2}]$	[3, -4]

Table 32: Wyckoff bond: 2b@2k

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

Table 33: Wyckoff bond: 4c@2k

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

\* Wyckoff site: 2l, site symmetry: 2

Table 34: Wyckoff bond: 2a@2l

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, y, \frac{1}{2}]$	[1, -2]
2	$[-X, 0, -Z]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	[3, -4]

Table 35: Wyckoff bond: 2b@21

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

Table 36: Wyckoff bond: 4c@21

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

\* Wyckoff site: 2m, site symmetry: m

Table 37: Wyckoff bond: 2a@2m

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	$[1, 4]$
2	$[-X, 0, -Z]$	$[-x, 0, -z]$	$[2, 3]$

Table 38: Wyckoff bond: 2b@2m

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, z]$	$[1, -4]$
2	$[0, Y, 0]$	$[-x, 0, -z]$	$[2, -3]$

Table 39: Wyckoff bond: 4c@2m

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, z]$	$[1]$
2	$[-X, Y, -Z]$	$[-x, 0, -z]$	$[2]$
3	$[-X, -Y, -Z]$	$[-x, 0, -z]$	$[3]$
4	$[X, -Y, Z]$	$[x, 0, z]$	$[4]$

\* Wyckoff site: 2n, site symmetry: m

Table 40: Wyckoff bond: 2a@2n

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, \frac{1}{2}, z]$	$[1, 4]$
2	$[-X, 0, -Z]$	$[-x, \frac{1}{2}, -z]$	$[2, 3]$

Table 41: Wyckoff bond: 2b@2n

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, \frac{1}{2}, z]$	$[1, -4]$
2	$[0, Y, 0]$	$[-x, \frac{1}{2}, -z]$	$[2, -3]$

Table 42: Wyckoff bond: 4c@2n

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

\* Wyckoff site: 4o, site symmetry: 1

Table 43: Wyckoff bond: 4a@4o

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	$[1]$
2	$[-X, Y, -Z]$	$[-x, y, -z]$	$[2]$
3	$[-X, -Y, -Z]$	$[-x, -y, -z]$	$[3]$
4	$[X, -Y, Z]$	$[x, -y, z]$	$[4]$