

SG No. 12 C_{2h}^3 $C2/m$ (b-axis setting) [monoclinic]

* plus set: $+ [0, 0, 0], + [\frac{1}{2}, \frac{1}{2}, 0]$

* Wyckoff site: 2a, site symmetry: $2/m$

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 4c@2a

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

* Wyckoff site: 2b, site symmetry: $2/m$

Table 4: Wyckoff bond: 2a@2b

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

Table 5: Wyckoff bond: 2b@2b

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

Table 6: Wyckoff bond: 4c@2b

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: 2c, site symmetry: 2/m

Table 7: Wyckoff bond: 2a@2c

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

Table 8: Wyckoff bond: 2b@2c

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

Table 9: Wyckoff bond: 4c@2c

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: 2d, site symmetry: 2/m

Table 10: Wyckoff bond: 2a@2d

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

Table 11: Wyckoff bond: 2b@2d

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

Table 12: Wyckoff bond: 4c@2d

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: 4e, site symmetry: -1

Table 13: Wyckoff bond: **4a@4e**

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

* Wyckoff site: **4f**, site symmetry: -1

Table 14: Wyckoff bond: **4a@4f**

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

* Wyckoff site: **4g**, site symmetry: 2

Table 15: Wyckoff bond: **4a@4g**

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

Table 16: Wyckoff bond: **4b@4g**

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

Table 17: Wyckoff bond: **8c@4g**

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: **4h**, site symmetry: 2

Table 18: Wyckoff bond: 4a@4h

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 19: Wyckoff bond: 4b@4h

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 20: Wyckoff bond: 8c@4h

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: 4i, site symmetry: m

Table 21: Wyckoff bond: 4a@4i

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

Table 22: Wyckoff bond: 4b@4i

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

Table 23: Wyckoff bond: $8c@4i$

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: $8j$, site symmetry: 1

Table 24: Wyckoff bond: $8a@8j$

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]