

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]