

SG No. 23 D_2^8 $I222$ [orthorhombic]

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

* Wyckoff site: 2a, site symmetry: 222

Table 1: Wyckoff bond: 2a@2a

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

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: 2c@2a

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

Table 4: Wyckoff bond: 4d@2a

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

Table 5: Wyckoff bond: 4e@2a

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

Table 6: Wyckoff bond: 4f@2a

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

Table 7: Wyckoff bond: 8g@2a

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

* Wyckoff site: 2b, site symmetry: 222

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 2b@2b

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

Table 10: Wyckoff bond: 2c@2b

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

Table 11: Wyckoff bond: 4d@2b

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

Table 12: Wyckoff bond: 4e@2b

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

Table 13: Wyckoff bond: 4f@2b

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

Table 14: Wyckoff bond: 8g@2b

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

* Wyckoff site: 2c, site symmetry: 222

Table 15: Wyckoff bond: 2a@2c

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

Table 16: Wyckoff bond: 2b@2c

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

Table 17: Wyckoff bond: 2c@2c

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

Table 18: Wyckoff bond: 4d@2c

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

Table 19: Wyckoff bond: 4e@2c

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

Table 20: Wyckoff bond: 4f@2c

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

Table 21: Wyckoff bond: 8g@2c

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

* Wyckoff site: 2d, site symmetry: 222

Table 22: Wyckoff bond: 2a@2d

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

Table 23: Wyckoff bond: 2b@2d

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

Table 24: Wyckoff bond: 2c@2d

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

Table 25: Wyckoff bond: 4d@2d

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

Table 26: Wyckoff bond: 4e@2d

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

Table 27: Wyckoff bond: 4f@2d

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

Table 28: Wyckoff bond: 8g@2d

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

* Wyckoff site: 4e, site symmetry: 2..

Table 29: Wyckoff bond: 4a@4e

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

Table 30: Wyckoff bond: 4b@4e

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

Table 31: Wyckoff bond: 8c@4e

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

* Wyckoff site: 4f, site symmetry: 2..

Table 32: Wyckoff bond: 4a@4f

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

Table 33: Wyckoff bond: 4b@4f

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

Table 34: Wyckoff bond: 8c@4f

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

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

Table 35: Wyckoff bond: 4a@4g

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

Table 36: Wyckoff bond: 4b@4g

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

Table 37: 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 38: Wyckoff bond: 4a@4h

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

Table 39: Wyckoff bond: 4b@4h

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

Table 40: Wyckoff bond: 8c@4h

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: 4i, site symmetry: . . 2

Table 41: Wyckoff bond: 4a@4i

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

Table 42: Wyckoff bond: 4b@4i

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

Table 43: Wyckoff bond: 8c@4i

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

* Wyckoff site: 4j, site symmetry: . . 2

Table 44: Wyckoff bond: 4a@4j

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

Table 45: Wyckoff bond: 4b@4j

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

Table 46: Wyckoff bond: 8c@4j

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

* Wyckoff site: 8k, site symmetry: 1

Table 47: Wyckoff bond: 8a@8k

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]