

SG No. 22 D_2^7 $F222$ [orthorhombic]

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

* Wyckoff site: 4a, site symmetry: 222

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 4b@4a

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

Table 3: Wyckoff bond: 4c@4a

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

Table 4: Wyckoff bond: 8d@4a

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: 8e@4a

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: 8f@4a

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: 16g@4a

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: 4b, site symmetry: 222

Table 8: Wyckoff bond: 4a@4b

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

Table 9: Wyckoff bond: 4b@4b

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

Table 10: Wyckoff bond: 4c@4b

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

Table 11: Wyckoff bond: 8d@4b

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 12: Wyckoff bond: 8e@4b

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 13: Wyckoff bond: 8f@4b

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 14: Wyckoff bond: 16g@4b

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: 4c, site symmetry: 222

Table 15: Wyckoff bond: 4a@4c

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

Table 16: Wyckoff bond: 4b@4c

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

Table 17: Wyckoff bond: 4c@4c

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

Table 18: Wyckoff bond: 8d@4c

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

Table 19: Wyckoff bond: 8e@4c

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

Table 20: Wyckoff bond: 8f@4c

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

Table 21: Wyckoff bond: 16g@4c

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

* Wyckoff site: 4d, site symmetry: 222

Table 22: Wyckoff bond: 4a@4d

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

Table 23: Wyckoff bond: 4b@4d

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

Table 24: Wyckoff bond: 4c@4d

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

Table 25: Wyckoff bond: 8d@4d

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

Table 26: Wyckoff bond: 8e@4d

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

Table 27: Wyckoff bond: 8f@4d

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

Table 28: Wyckoff bond: 16g@4d

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

* Wyckoff site: 8e, site symmetry: 2..

Table 29: Wyckoff bond: 8a@8e

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: 8b@8e

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: 16c@8e

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: 8f, site symmetry: .2.

Table 32: Wyckoff bond: 8a@8f

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

Table 33: Wyckoff bond: 8b@8f

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

Table 34: Wyckoff bond: 16c@8f

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: 8g, site symmetry: ..2

Table 35: Wyckoff bond: 8a@8g

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

Table 36: Wyckoff bond: 8b@8g

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

Table 37: Wyckoff bond: 16c@8g

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: 8h, site symmetry: ...2

Table 38: Wyckoff bond: 8a@8h

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

Table 39: Wyckoff bond: 8b@8h

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

Table 40: Wyckoff bond: 16c@8h

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

* Wyckoff site: 8i, site symmetry: .2.

Table 41: Wyckoff bond: 8a@8i

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

Table 42: Wyckoff bond: 8b@8i

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

Table 43: Wyckoff bond: 16c@8i

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

* Wyckoff site: 8j, site symmetry: 2..

Table 44: Wyckoff bond: 8a@8j

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

Table 45: Wyckoff bond: 8b@8j

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

Table 46: Wyckoff bond: 16c@8j

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

* Wyckoff site: 16k, site symmetry: 1

Table 47: Wyckoff bond: 16a@16k

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]