

SG No. 66 D_{2h}^{20} $Cccm$ [orthorhombic]

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

* Wyckoff site: 4a, site symmetry: 222

Table 1: Wyckoff bond: 4a@4a

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, \frac{1}{4}]$	$[1, 2, -3, -4]$
2	$[0, 0, -Z]$	$[0, 0, \frac{3}{4}]$	$[5, 6, -7, -8]$

Table 2: Wyckoff bond: 4b@4a

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, \frac{1}{4}]$	$[1, -2, 3, -4]$
2	$[0, -Y, 0]$	$[0, 0, \frac{3}{4}]$	$[5, -6, 7, -8]$

Table 3: Wyckoff bond: 4c@4a

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, \frac{1}{4}]$	$[1, -2, -3, 4]$
2	$[-X, 0, 0]$	$[0, 0, \frac{3}{4}]$	$[5, -6, -7, 8]$

Table 4: Wyckoff bond: 8d@4a

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, \frac{1}{4}]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, 0, \frac{1}{4}]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[0, 0, \frac{3}{4}]$	$[5, -6]$
4	$[X, -Y, 0]$	$[0, 0, \frac{3}{4}]$	$[7, -8]$

Table 5: Wyckoff bond: 8e@4a

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, \frac{1}{4}]$	$[1, -3]$
2	$[-X, 0, Z]$	$[0, 0, \frac{1}{4}]$	$[2, -4]$
3	$[-X, 0, -Z]$	$[0, 0, \frac{3}{4}]$	$[5, -7]$
4	$[X, 0, -Z]$	$[0, 0, \frac{3}{4}]$	$[6, -8]$

Table 6: Wyckoff bond: 8f@4a

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, \frac{1}{4}]$	$[1, -4]$
2	$[0, -Y, Z]$	$[0, 0, \frac{1}{4}]$	$[2, -3]$
3	$[0, -Y, -Z]$	$[0, 0, \frac{3}{4}]$	$[5, -8]$
4	$[0, Y, -Z]$	$[0, 0, \frac{3}{4}]$	$[6, -7]$

Table 7: Wyckoff bond: 16g@4a

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{4}]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, \frac{1}{4}]$	$[2]$
3	$[-X, Y, -Z]$	$[0, 0, \frac{1}{4}]$	$[3]$
4	$[X, -Y, -Z]$	$[0, 0, \frac{1}{4}]$	$[4]$
5	$[-X, -Y, -Z]$	$[0, 0, \frac{3}{4}]$	$[5]$
6	$[X, Y, -Z]$	$[0, 0, \frac{3}{4}]$	$[6]$
7	$[X, -Y, Z]$	$[0, 0, \frac{3}{4}]$	$[7]$
8	$[-X, Y, Z]$	$[0, 0, \frac{3}{4}]$	$[8]$

* Wyckoff site: 4b, site symmetry: 222

Table 8: Wyckoff bond: 4a@4b

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, -3, -4]$
2	$[0, 0, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[5, 6, -7, -8]$

Table 9: Wyckoff bond: 4b@4b

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, -2, 3, -4]$
2	$[0, -Y, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[5, -6, 7, -8]$

Table 10: Wyckoff bond: 4c@4b

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, -2, -3, 4]$
2	$[-X, 0, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[5, -6, -7, 8]$

Table 11: Wyckoff bond: 8d@4b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[1,-2]
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[3,-4]
3	$[-X, -Y, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[5,-6]
4	$[X, -Y, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[7,-8]

Table 12: Wyckoff bond: 8e@4b

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[1,-3]
2	$[-X, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2,-4]
3	$[-X, 0, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[5,-7]
4	$[X, 0, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[6,-8]

Table 13: Wyckoff bond: 8f@4b

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[1,-4]
2	$[0, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2,-3]
3	$[0, -Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[5,-8]
4	$[0, Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[6,-7]

Table 14: Wyckoff bond: 16g@4b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2]
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[3]
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[4]
5	$[-X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[5]
6	$[X, Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[6]
7	$[X, -Y, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[7]
8	$[-X, Y, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[8]

* Wyckoff site: 4c, site symmetry: . . 2/m

Table 15: Wyckoff bond: 4a@4c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 16: Wyckoff bond: 4b@4c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	$[1, 2, -5, -6]$
2	$[0, 0, -Z]$	$[0, 0, \frac{1}{2}]$	$[3, 4, -7, -8]$

Table 17: Wyckoff bond: 8c@4c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[0, 0, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[4, -8]$

* Wyckoff site: 4d, site symmetry: $\dots 2/m$

Table 18: Wyckoff bond: 4a@4d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 19: Wyckoff bond: 4b@4d

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, 0]$	$[1, 2, -5, -6]$
2	$[0, 0, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 4, -7, -8]$

Table 20: Wyckoff bond: 8c@4d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, -8]$

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

Table 21: Wyckoff bond: 4a@4e

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 22: Wyckoff bond: 4b@4e

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 2, -5, -6]$
2	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[3, 4, -7, -8]$

Table 23: Wyckoff bond: 8c@4e

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[4, -8]$

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

Table 24: Wyckoff bond: 4a@4f

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 25: Wyckoff bond: 4b@4f

No.	vector	center	mapping
1	[0, 0, Z]	$[\frac{1}{4}, \frac{3}{4}, 0]$	[1, 2, -5, -6]
2	[0, 0, -Z]	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[3, 4, -7, -8]

Table 26: Wyckoff bond: 8c@4f

No.	vector	center	mapping
1	[X, Y, Z]	$[\frac{1}{4}, \frac{3}{4}, 0]$	[1, -5]
2	[-X, -Y, Z]	$[\frac{1}{4}, \frac{3}{4}, 0]$	[2, -6]
3	[-X, Y, -Z]	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[3, -7]
4	[X, -Y, -Z]	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[4, -8]

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

Table 27: Wyckoff bond: 8a@8g

No.	vector	center	mapping
1	[0, Y, Z]	$[x, 0, \frac{1}{4}]$	[1, -4]
2	[0, -Y, Z]	$[-x, 0, \frac{1}{4}]$	[2, -3]
3	[0, -Y, -Z]	$[-x, 0, \frac{3}{4}]$	[5, -8]
4	[0, Y, -Z]	$[x, 0, \frac{3}{4}]$	[6, -7]

Table 28: Wyckoff bond: 8b@8g

No.	vector	center	mapping
1	[X, 0, 0]	$[x, 0, \frac{1}{4}]$	[1, 4]
2	[-X, 0, 0]	$[-x, 0, \frac{1}{4}]$	[2, 3]
3	[-X, 0, 0]	$[-x, 0, \frac{3}{4}]$	[5, 8]
4	[X, 0, 0]	$[x, 0, \frac{3}{4}]$	[6, 7]

Table 29: Wyckoff bond: 16c@8g

No.	vector	center	mapping
1	[X, Y, Z]	$[x, 0, \frac{1}{4}]$	[1]
2	[-X, -Y, Z]	$[-x, 0, \frac{1}{4}]$	[2]
3	[-X, Y, -Z]	$[-x, 0, \frac{1}{4}]$	[3]
4	[X, -Y, -Z]	$[x, 0, \frac{1}{4}]$	[4]
5	[-X, -Y, -Z]	$[-x, 0, \frac{3}{4}]$	[5]

continued ...

Table 29

No.	vector	center	mapping
6	$[X, Y, -Z]$	$[x, 0, \frac{3}{4}]$	[6]
7	$[X, -Y, Z]$	$[x, 0, \frac{3}{4}]$	[7]
8	$[-X, Y, Z]$	$[-x, 0, \frac{3}{4}]$	[8]

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

Table 30: Wyckoff bond: 8a@8h

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, \frac{1}{4}]$	[1,-3]
2	$[-X, 0, Z]$	$[0, -y, \frac{1}{4}]$	[2,-4]
3	$[-X, 0, -Z]$	$[0, -y, \frac{3}{4}]$	[5,-7]
4	$[X, 0, -Z]$	$[0, y, \frac{3}{4}]$	[6,-8]

Table 31: Wyckoff bond: 8b@8h

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, \frac{1}{4}]$	[1,3]
2	$[0, -Y, 0]$	$[0, -y, \frac{1}{4}]$	[2,4]
3	$[0, -Y, 0]$	$[0, -y, \frac{3}{4}]$	[5,7]
4	$[0, Y, 0]$	$[0, y, \frac{3}{4}]$	[6,8]

Table 32: Wyckoff bond: 16c@8h

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[0, -y, \frac{1}{4}]$	[2]
3	$[-X, Y, -Z]$	$[0, y, \frac{1}{4}]$	[3]
4	$[X, -Y, -Z]$	$[0, -y, \frac{1}{4}]$	[4]
5	$[-X, -Y, -Z]$	$[0, -y, \frac{3}{4}]$	[5]
6	$[X, Y, -Z]$	$[0, y, \frac{3}{4}]$	[6]
7	$[X, -Y, Z]$	$[0, -y, \frac{3}{4}]$	[7]
8	$[-X, Y, Z]$	$[0, y, \frac{3}{4}]$	[8]

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

Table 33: Wyckoff bond: 8a@8i

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, 0, \frac{1}{2} - z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[0, 0, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[0, 0, z + \frac{1}{2}]$	$[7, -8]$

Table 34: Wyckoff bond: 8b@8i

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2]$
2	$[0, 0, -Z]$	$[0, 0, \frac{1}{2} - z]$	$[3, 4]$
3	$[0, 0, -Z]$	$[0, 0, -z]$	$[5, 6]$
4	$[0, 0, Z]$	$[0, 0, z + \frac{1}{2}]$	$[7, 8]$

Table 35: Wyckoff bond: 16c@8i

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, z]$	$[2]$
3	$[-X, Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	$[3]$
4	$[X, -Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	$[4]$
5	$[-X, -Y, -Z]$	$[0, 0, -z]$	$[5]$
6	$[X, Y, -Z]$	$[0, 0, -z]$	$[6]$
7	$[X, -Y, Z]$	$[0, 0, z + \frac{1}{2}]$	$[7]$
8	$[-X, Y, Z]$	$[0, 0, z + \frac{1}{2}]$	$[8]$

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

Table 36: Wyckoff bond: 8a@8j

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[0, \frac{1}{2}, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[7, -8]$

Table 37: Wyckoff bond: 8b@8j

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	[1, 2]
2	$[0, 0, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[3, 4]
3	$[0, 0, -Z]$	$[0, \frac{1}{2}, -z]$	[5, 6]
4	$[0, 0, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[7, 8]

Table 38: Wyckoff bond: 16c@8j

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	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[4]
5	$[-X, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	[5]
6	$[X, Y, -Z]$	$[0, \frac{1}{2}, -z]$	[6]
7	$[X, -Y, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[8]

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

Table 39: Wyckoff bond: 8a@8k

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1, -2]
2	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3, -4]
3	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5, -6]
4	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7, -8]

Table 40: Wyckoff bond: 8b@8k

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1, 2]
2	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3, 4]
3	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5, 6]
4	$[0, 0, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7, 8]

Table 41: Wyckoff bond: 16c@8k

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	$[-X, Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[4]
5	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5]
6	$[X, Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[6]
7	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[8]

* Wyckoff site: 81, site symmetry: . .m

Table 42: Wyckoff bond: 8a@81

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	[1,6]
2	$[-X, -Y, 0]$	$[-x, -y, 0]$	[2,5]
3	$[-X, Y, 0]$	$[-x, y, \frac{1}{2}]$	[3,8]
4	$[X, -Y, 0]$	$[x, -y, \frac{1}{2}]$	[4,7]

Table 43: Wyckoff bond: 8b@81

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, 0]$	[1,-6]
2	$[0, 0, Z]$	$[-x, -y, 0]$	[2,-5]
3	$[0, 0, -Z]$	$[-x, y, \frac{1}{2}]$	[3,-8]
4	$[0, 0, -Z]$	$[x, -y, \frac{1}{2}]$	[4,-7]

Table 44: Wyckoff bond: 16c@81

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, 0]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, \frac{1}{2}]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, \frac{1}{2}]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, 0]$	[5]
6	$[X, Y, -Z]$	$[x, y, 0]$	[6]
7	$[X, -Y, Z]$	$[x, -y, \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[-x, y, \frac{1}{2}]$	[8]

* Wyckoff site: 16m, site symmetry: 1

Table 45: Wyckoff bond: 16a@16m

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, \frac{1}{2} - z]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[5]
6	$[X, Y, -Z]$	$[x, y, -z]$	[6]
7	$[X, -Y, Z]$	$[x, -y, z + \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[-x, y, z + \frac{1}{2}]$	[8]