

SG No. 116  $D_{2d}^6$   $P\bar{4}c2$  [ tetragonal ]

\* plus set: + [0, 0, 0]

\* Wyckoff site: 2a, site symmetry: 2.22

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 2c@2a

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

Table 4: Wyckoff bond: 4d@2a

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

Table 5: Wyckoff bond: 4e@2a

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

Table 6: Wyckoff bond: 4f@2a

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

Table 7: Wyckoff bond: 8g@2a

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

\* Wyckoff site: 2b, site symmetry: 2.22

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 2b@2b

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

Table 10: Wyckoff bond: 2c@2b

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

Table 11: Wyckoff bond: 4d@2b

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

Table 12: Wyckoff bond: 4e@2b

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

Table 13: Wyckoff bond: 4f@2b

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

Table 14: Wyckoff bond: 8g@2b

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

\* Wyckoff site: 2c, site symmetry: -4..

Table 15: Wyckoff bond: 2a@2c

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

Table 16: Wyckoff bond: 4b@2c

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

Table 17: Wyckoff bond: 8c@2c

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

\* Wyckoff site: 2d, site symmetry: -4..

Table 18: Wyckoff bond: 2a@2d

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

Table 19: Wyckoff bond: 4b@2d

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

*continued ...*

Table 19

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

Table 20: Wyckoff bond: 8c@2d

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

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

Table 21: Wyckoff bond: 4a@4e

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

Table 22: Wyckoff bond: 4b@4e

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

Table 23: Wyckoff bond: 8c@4e

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

*continued ...*

Table 23

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

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

Table 24: Wyckoff bond: 4a@4f

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

Table 25: Wyckoff bond: 4b@4f

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

Table 26: Wyckoff bond: 8c@4f

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

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

Table 27: Wyckoff bond: 4a@4g

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

Table 28: Wyckoff bond: 4b@4g

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

Table 29: Wyckoff bond: 8c@4g

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

\* Wyckoff site: 4h, site symmetry: 2..

Table 30: Wyckoff bond: 4a@4h

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

Table 31: Wyckoff bond: 4b@4h

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

Table 32: Wyckoff bond: 8c@4h

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

\* Wyckoff site: 4i, site symmetry: 2..

Table 33: Wyckoff bond: 4a@4i

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

Table 34: Wyckoff bond: 4b@4i

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

Table 35: Wyckoff bond: 8c@4i

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

\* Wyckoff site: 8j, site symmetry: 1

Table 36: 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	$[Y, -X, -Z]$	$[y, -x, -z]$	[3]
4	$[-Y, X, -Z]$	$[-y, x, -z]$	[4]
5	$[X, -Y, Z]$	$[x, -y, z + \frac{1}{2}]$	[5]
6	$[-X, Y, Z]$	$[-x, y, z + \frac{1}{2}]$	[6]
7	$[Y, X, -Z]$	$[y, x, \frac{1}{2} - z]$	[7]
8	$[-Y, -X, -Z]$	$[-y, -x, \frac{1}{2} - z]$	[8]