

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

Table 19: Wyckoff bond: 4b@2d

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

*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:  $\bar{3}2$

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:  $\bar{3}2$

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:  $2\bar{1}$

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]