

PG No. 15 D_{4h} 4/mmm [tetragonal]

* Wyckoff site: 2a, site symmetry: 4mm

Table 1: Wyckoff bond: 2a@2a

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	[1,2,3,4,13,14,15,16]
2	[0, 0, -Z]	[0, 0, -z]	[5,6,7,8,9,10,11,12]

Table 2: Wyckoff bond: 4b@2a

No.	vector	center	mapping
1	[X, 0, 0]	[0, 0, z]	[1,-2,13,-14]
2	[0, X, 0]	[0, 0, z]	[3,-4,-15,16]
3	[-X, 0, 0]	[0, 0, -z]	[5,-6,9,-10]
4	[0, X, 0]	[0, 0, -z]	[7,-8,-11,12]

Table 3: Wyckoff bond: 4c@2a

No.	vector	center	mapping
1	[X, X, 0]	[0, 0, z]	[1,-2,-15,16]
2	[-X, X, 0]	[0, 0, z]	[3,-4,-13,14]
3	[-X, X, 0]	[0, 0, -z]	[5,-6,-11,12]
4	[X, X, 0]	[0, 0, -z]	[7,-8,-9,10]

Table 4: Wyckoff bond: 8d@2a

No.	vector	center	mapping
1	[X, 0, Z]	[0, 0, z]	[1,13]
2	[-X, 0, Z]	[0, 0, z]	[2,14]
3	[0, X, Z]	[0, 0, z]	[3,16]
4	[0, -X, Z]	[0, 0, z]	[4,15]
5	[-X, 0, -Z]	[0, 0, -z]	[5,9]
6	[X, 0, -Z]	[0, 0, -z]	[6,10]
7	[0, X, -Z]	[0, 0, -z]	[7,12]
8	[0, -X, -Z]	[0, 0, -z]	[8,11]

Table 5: Wyckoff bond: 8e@2a

No.	vector	center	mapping
1	[X, X, Z]	[0, 0, z]	[1, 16]
2	[-X, -X, Z]	[0, 0, z]	[2, 15]
3	[-X, X, Z]	[0, 0, z]	[3, 14]
4	[X, -X, Z]	[0, 0, z]	[4, 13]
5	[-X, X, -Z]	[0, 0, -z]	[5, 12]
6	[X, -X, -Z]	[0, 0, -z]	[6, 11]
7	[X, X, -Z]	[0, 0, -z]	[7, 10]
8	[-X, -X, -Z]	[0, 0, -z]	[8, 9]

Table 6: Wyckoff bond: 8f@2a

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]	[5, -6]
4	[Y, X, 0]	[0, 0, -z]	[7, -8]
5	[-X, -Y, 0]	[0, 0, -z]	[9, -10]
6	[Y, -X, 0]	[0, 0, -z]	[11, -12]
7	[X, -Y, 0]	[0, 0, z]	[13, -14]
8	[-Y, -X, 0]	[0, 0, z]	[15, -16]

Table 7: Wyckoff bond: 16g@2a

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]	[5]
6	[X, -Y, -Z]	[0, 0, -z]	[6]
7	[Y, X, -Z]	[0, 0, -z]	[7]
8	[-Y, -X, -Z]	[0, 0, -z]	[8]
9	[-X, -Y, -Z]	[0, 0, -z]	[9]
10	[X, Y, -Z]	[0, 0, -z]	[10]
11	[Y, -X, -Z]	[0, 0, -z]	[11]
12	[-Y, X, -Z]	[0, 0, -z]	[12]
13	[X, -Y, Z]	[0, 0, z]	[13]
14	[-X, Y, Z]	[0, 0, z]	[14]
15	[-Y, -X, Z]	[0, 0, z]	[15]
16	[Y, X, Z]	[0, 0, z]	[16]

* Wyckoff site: **4b**, site symmetry: **m.m2**

Table 8: Wyckoff bond: **4a@4b**

No.	vector	center	mapping
1	[$X, X, 0$]	[$x, x, 0$]	[1,7,10,16]
2	[$-X, -X, 0$]	[$-x, -x, 0$]	[2,8,9,15]
3	[$-X, X, 0$]	[$-x, x, 0$]	[3,5,12,14]
4	[$X, -X, 0$]	[$x, -x, 0$]	[4,6,11,13]

Table 9: Wyckoff bond: **4b@4b**

No.	vector	center	mapping
1	[$X, -X, 0$]	[$x, x, 0$]	[1,-7,10,-16]
2	[$-X, X, 0$]	[$-x, -x, 0$]	[2,-8,9,-15]
3	[$X, X, 0$]	[$-x, x, 0$]	[3,-5,12,-14]
4	[$-X, -X, 0$]	[$x, -x, 0$]	[4,-6,11,-13]

Table 10: Wyckoff bond: **4c@4b**

No.	vector	center	mapping
1	[0, 0, Z]	[$x, x, 0$]	[1,-7,-10,16]
2	[0, 0, Z]	[$-x, -x, 0$]	[2,-8,-9,15]
3	[0, 0, Z]	[$-x, x, 0$]	[3,-5,-12,14]
4	[0, 0, Z]	[$x, -x, 0$]	[4,-6,-11,13]

Table 11: Wyckoff bond: **8d@4b**

No.	vector	center	mapping
1	[X, X, Z]	[$x, x, 0$]	[1,16]
2	[$-X, -X, Z$]	[$-x, -x, 0$]	[2,15]
3	[$-X, X, Z$]	[$-x, x, 0$]	[3,14]
4	[$X, -X, Z$]	[$x, -x, 0$]	[4,13]
5	[$-X, X, -Z$]	[$-x, x, 0$]	[5,12]
6	[$X, -X, -Z$]	[$x, -x, 0$]	[6,11]
7	[$X, X, -Z$]	[$x, x, 0$]	[7,10]
8	[$-X, -X, -Z$]	[$-x, -x, 0$]	[8,9]

Table 12: Wyckoff bond: 8e@4b

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, x, 0]$	[1,-7]
2	$[-X, X, Z]$	$[-x, -x, 0]$	[2,-8]
3	$[X, X, Z]$	$[-x, x, 0]$	[3,-5]
4	$[-X, -X, Z]$	$[x, -x, 0]$	[4,-6]
5	$[-X, X, -Z]$	$[-x, -x, 0]$	[9,-15]
6	$[X, -X, -Z]$	$[x, x, 0]$	[10,-16]
7	$[-X, -X, -Z]$	$[x, -x, 0]$	[11,-13]
8	$[X, X, -Z]$	$[-x, x, 0]$	[12,-14]

Table 13: Wyckoff bond: 8f@4b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, x, 0]$	[1,10]
2	$[-X, -Y, 0]$	$[-x, -x, 0]$	[2,9]
3	$[-Y, X, 0]$	$[-x, x, 0]$	[3,12]
4	$[Y, -X, 0]$	$[x, -x, 0]$	[4,11]
5	$[-X, Y, 0]$	$[-x, x, 0]$	[5,14]
6	$[X, -Y, 0]$	$[x, -x, 0]$	[6,13]
7	$[Y, X, 0]$	$[x, x, 0]$	[7,16]
8	$[-Y, -X, 0]$	$[-x, -x, 0]$	[8,15]

Table 14: Wyckoff bond: 16g@4b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, 0]$	[1]
2	$[-X, -Y, Z]$	$[-x, -x, 0]$	[2]
3	$[-Y, X, Z]$	$[-x, x, 0]$	[3]
4	$[Y, -X, Z]$	$[x, -x, 0]$	[4]
5	$[-X, Y, -Z]$	$[-x, x, 0]$	[5]
6	$[X, -Y, -Z]$	$[x, -x, 0]$	[6]
7	$[Y, X, -Z]$	$[x, x, 0]$	[7]
8	$[-Y, -X, -Z]$	$[-x, -x, 0]$	[8]
9	$[-X, -Y, -Z]$	$[-x, -x, 0]$	[9]
10	$[X, Y, -Z]$	$[x, x, 0]$	[10]
11	$[Y, -X, -Z]$	$[x, -x, 0]$	[11]
12	$[-Y, X, -Z]$	$[-x, x, 0]$	[12]
13	$[X, -Y, Z]$	$[x, -x, 0]$	[13]
14	$[-X, Y, Z]$	$[-x, x, 0]$	[14]
15	$[-Y, -X, Z]$	$[-x, -x, 0]$	[15]
16	$[Y, X, Z]$	$[x, x, 0]$	[16]

* Wyckoff site: 4c, site symmetry: m2m.

Table 15: Wyckoff bond: 4a@4c

No.	vector	center	mapping
1	[X, 0, 0]	[x, 0, 0]	[1, 6, 10, 13]
2	[-X, 0, 0]	[-x, 0, 0]	[2, 5, 9, 14]
3	[0, X, 0]	[0, x, 0]	[3, 7, 12, 16]
4	[0, -X, 0]	[0, -x, 0]	[4, 8, 11, 15]

Table 16: Wyckoff bond: 4b@4c

No.	vector	center	mapping
1	[0, X, 0]	[x, 0, 0]	[1, -6, 10, -13]
2	[0, -X, 0]	[-x, 0, 0]	[2, -5, 9, -14]
3	[-X, 0, 0]	[0, x, 0]	[3, -7, 12, -16]
4	[X, 0, 0]	[0, -x, 0]	[4, -8, 11, -15]

Table 17: Wyckoff bond: 4c@4c

No.	vector	center	mapping
1	[0, 0, Z]	[x, 0, 0]	[1, -6, -10, 13]
2	[0, 0, Z]	[-x, 0, 0]	[2, -5, -9, 14]
3	[0, 0, Z]	[0, x, 0]	[3, -7, -12, 16]
4	[0, 0, Z]	[0, -x, 0]	[4, -8, -11, 15]

Table 18: Wyckoff bond: 8d@4c

No.	vector	center	mapping
1	[X, 0, Z]	[x, 0, 0]	[1, 13]
2	[-X, 0, Z]	[-x, 0, 0]	[2, 14]
3	[0, X, Z]	[0, x, 0]	[3, 16]
4	[0, -X, Z]	[0, -x, 0]	[4, 15]
5	[-X, 0, -Z]	[-x, 0, 0]	[5, 9]
6	[X, 0, -Z]	[x, 0, 0]	[6, 10]
7	[0, X, -Z]	[0, x, 0]	[7, 12]
8	[0, -X, -Z]	[0, -x, 0]	[8, 11]

Table 19: Wyckoff bond: 8e@4c

No.	vector	center	mapping
1	[0, X, Z]	[x, 0, 0]	[1,-6]
2	[0, -X, Z]	[-x, 0, 0]	[2,-5]
3	[-X, 0, Z]	[0, x, 0]	[3,-7]
4	[X, 0, Z]	[0, -x, 0]	[4,-8]
5	[0, -X, -Z]	[-x, 0, 0]	[9,-14]
6	[0, X, -Z]	[x, 0, 0]	[10,-13]
7	[X, 0, -Z]	[0, -x, 0]	[11,-15]
8	[-X, 0, -Z]	[0, x, 0]	[12,-16]

Table 20: Wyckoff bond: 8f@4c

No.	vector	center	mapping
1	[X, Y, 0]	[x, 0, 0]	[1,10]
2	[-X, -Y, 0]	[-x, 0, 0]	[2,9]
3	[-Y, X, 0]	[0, x, 0]	[3,12]
4	[Y, -X, 0]	[0, -x, 0]	[4,11]
5	[-X, Y, 0]	[-x, 0, 0]	[5,14]
6	[X, -Y, 0]	[x, 0, 0]	[6,13]
7	[Y, X, 0]	[0, x, 0]	[7,16]
8	[-Y, -X, 0]	[0, -x, 0]	[8,15]

Table 21: Wyckoff bond: 16g@4c

No.	vector	center	mapping
1	[X, Y, Z]	[x, 0, 0]	[1]
2	[-X, -Y, Z]	[-x, 0, 0]	[2]
3	[-Y, X, Z]	[0, x, 0]	[3]
4	[Y, -X, Z]	[0, -x, 0]	[4]
5	[-X, Y, -Z]	[-x, 0, 0]	[5]
6	[X, -Y, -Z]	[x, 0, 0]	[6]
7	[Y, X, -Z]	[0, x, 0]	[7]
8	[-Y, -X, -Z]	[0, -x, 0]	[8]
9	[-X, -Y, -Z]	[-x, 0, 0]	[9]
10	[X, Y, -Z]	[x, 0, 0]	[10]
11	[Y, -X, -Z]	[0, -x, 0]	[11]
12	[-Y, X, -Z]	[0, x, 0]	[12]
13	[X, -Y, Z]	[x, 0, 0]	[13]
14	[-X, Y, Z]	[-x, 0, 0]	[14]
15	[-Y, -X, Z]	[0, -x, 0]	[15]
16	[Y, X, Z]	[0, x, 0]	[16]

* Wyckoff site: 8d, site symmetry: m..

Table 22: Wyckoff bond: 8a@8d

No.	vector	center	mapping
1	[X, Y, 0]	[x, y, 0]	[1,10]
2	[-X, -Y, 0]	[-x, -y, 0]	[2,9]
3	[-Y, X, 0]	[-y, x, 0]	[3,12]
4	[Y, -X, 0]	[y, -x, 0]	[4,11]
5	[-X, Y, 0]	[-x, y, 0]	[5,14]
6	[X, -Y, 0]	[x, -y, 0]	[6,13]
7	[Y, X, 0]	[y, x, 0]	[7,16]
8	[-Y, -X, 0]	[-y, -x, 0]	[8,15]

Table 23: Wyckoff bond: 8b@8d

No.	vector	center	mapping
1	[0, 0, Z]	[x, y, 0]	[1,-10]
2	[0, 0, Z]	[-x, -y, 0]	[2,-9]
3	[0, 0, Z]	[-y, x, 0]	[3,-12]
4	[0, 0, Z]	[y, -x, 0]	[4,-11]
5	[0, 0, -Z]	[-x, y, 0]	[5,-14]
6	[0, 0, -Z]	[x, -y, 0]	[6,-13]
7	[0, 0, -Z]	[y, x, 0]	[7,-16]
8	[0, 0, -Z]	[-y, -x, 0]	[8,-15]

Table 24: Wyckoff bond: 16c@8d

No.	vector	center	mapping
1	[X, Y, Z]	[x, y, 0]	[1]
2	[-X, -Y, Z]	[-x, -y, 0]	[2]
3	[-Y, X, Z]	[-y, x, 0]	[3]
4	[Y, -X, Z]	[y, -x, 0]	[4]
5	[-X, Y, -Z]	[-x, y, 0]	[5]
6	[X, -Y, -Z]	[x, -y, 0]	[6]
7	[Y, X, -Z]	[y, x, 0]	[7]
8	[-Y, -X, -Z]	[-y, -x, 0]	[8]
9	[-X, -Y, -Z]	[-x, -y, 0]	[9]
10	[X, Y, -Z]	[x, y, 0]	[10]
11	[Y, -X, -Z]	[y, -x, 0]	[11]
12	[-Y, X, -Z]	[-y, x, 0]	[12]
13	[X, -Y, Z]	[x, -y, 0]	[13]
14	[-X, Y, Z]	[-x, y, 0]	[14]
15	[-Y, -X, Z]	[-y, -x, 0]	[15]

continued ...

Table 24

No.	vector	center	mapping
16	[Y, X, Z]	[$y, x, 0$]	[16]

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

Table 25: Wyckoff bond: **8a@8e**

No.	vector	center	mapping
1	[X, X, Z]	[x, x, z]	[1, 16]
2	[$-X, -X, Z$]	[$-x, -x, z$]	[2, 15]
3	[$-X, X, Z$]	[$-x, x, z$]	[3, 14]
4	[$X, -X, Z$]	[$x, -x, z$]	[4, 13]
5	[$-X, X, -Z$]	[$-x, x, -z$]	[5, 12]
6	[$X, -X, -Z$]	[$x, -x, -z$]	[6, 11]
7	[$X, X, -Z$]	[$x, x, -z$]	[7, 10]
8	[$-X, -X, -Z$]	[$-x, -x, -z$]	[8, 9]

Table 26: Wyckoff bond: **8b@8e**

No.	vector	center	mapping
1	[$X, -X, 0$]	[x, x, z]	[1, 16]
2	[$-X, X, 0$]	[$-x, -x, z$]	[2, -15]
3	[$X, X, 0$]	[$-x, x, z$]	[3, -14]
4	[$-X, -X, 0$]	[$x, -x, z$]	[4, -13]
5	[$-X, -X, 0$]	[$-x, x, -z$]	[5, -12]
6	[$X, X, 0$]	[$x, -x, -z$]	[6, -11]
7	[$-X, X, 0$]	[$x, x, -z$]	[7, -10]
8	[$X, -X, 0$]	[$-x, -x, -z$]	[8, -9]

Table 27: Wyckoff bond: **16c@8e**

No.	vector	center	mapping
1	[X, Y, Z]	[x, x, z]	[1]
2	[$-X, -Y, Z$]	[$-x, -x, z$]	[2]
3	[$-Y, X, Z$]	[$-x, x, z$]	[3]
4	[$Y, -X, Z$]	[$x, -x, z$]	[4]
5	[$-X, Y, -Z$]	[$-x, x, -z$]	[5]
6	[$X, -Y, -Z$]	[$x, -x, -z$]	[6]
7	[$Y, X, -Z$]	[$x, x, -z$]	[7]
8	[$-Y, -X, -Z$]	[$-x, -x, -z$]	[8]
9	[$-X, -Y, -Z$]	[$-x, -x, -z$]	[9]

continued ...

Table 27

No.	vector	center	mapping
10	$[X, Y, -Z]$	$[x, x, -z]$	[10]
11	$[Y, -X, -Z]$	$[x, -x, -z]$	[11]
12	$[-Y, X, -Z]$	$[-x, x, -z]$	[12]
13	$[X, -Y, Z]$	$[x, -x, z]$	[13]
14	$[-X, Y, Z]$	$[-x, x, z]$	[14]
15	$[-Y, -X, Z]$	$[-x, -x, z]$	[15]
16	$[Y, X, Z]$	$[x, x, z]$	[16]

* Wyckoff site: 8f, site symmetry: .m.

Table 28: Wyckoff bond: 8a@8f

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	[1,13]
2	$[-X, 0, Z]$	$[-x, 0, z]$	[2,14]
3	$[0, X, Z]$	$[0, x, z]$	[3,16]
4	$[0, -X, Z]$	$[0, -x, z]$	[4,15]
5	$[-X, 0, -Z]$	$[-x, 0, -z]$	[5,9]
6	$[X, 0, -Z]$	$[x, 0, -z]$	[6,10]
7	$[0, X, -Z]$	$[0, x, -z]$	[7,12]
8	$[0, -X, -Z]$	$[0, -x, -z]$	[8,11]

Table 29: Wyckoff bond: 8b@8f

No.	vector	center	mapping
1	$[0, X, 0]$	$[x, 0, z]$	[1,-13]
2	$[0, -X, 0]$	$[-x, 0, z]$	[2,-14]
3	$[-X, 0, 0]$	$[0, x, z]$	[3,-16]
4	$[X, 0, 0]$	$[0, -x, z]$	[4,-15]
5	$[0, X, 0]$	$[-x, 0, -z]$	[5,-9]
6	$[0, -X, 0]$	$[x, 0, -z]$	[6,-10]
7	$[X, 0, 0]$	$[0, x, -z]$	[7,-12]
8	$[-X, 0, 0]$	$[0, -x, -z]$	[8,-11]

Table 30: Wyckoff bond: 16c@8f

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

continued ...

Table 30

No.	vector	center	mapping
4	[$Y, -X, Z$]	[$0, -x, z$]	[4]
5	[$-X, Y, -Z$]	[$-x, 0, -z$]	[5]
6	[$X, -Y, -Z$]	[$x, 0, -z$]	[6]
7	[$Y, X, -Z$]	[$0, x, -z$]	[7]
8	[$-Y, -X, -Z$]	[$0, -x, -z$]	[8]
9	[$-X, -Y, -Z$]	[$-x, 0, -z$]	[9]
10	[$X, Y, -Z$]	[$x, 0, -z$]	[10]
11	[$Y, -X, -Z$]	[$0, -x, -z$]	[11]
12	[$-Y, X, -Z$]	[$0, x, -z$]	[12]
13	[$X, -Y, Z$]	[$x, 0, z$]	[13]
14	[$-X, Y, Z$]	[$-x, 0, z$]	[14]
15	[$-Y, -X, Z$]	[$0, -x, z$]	[15]
16	[Y, X, Z]	[$0, x, z$]	[16]

* Wyckoff site: 16g, site symmetry: 1

Table 31: Wyckoff bond: 16a@16g

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	[$-X, Y, -Z$]	[$-x, y, -z$]	[5]
6	[$X, -Y, -Z$]	[$x, -y, -z$]	[6]
7	[$Y, X, -Z$]	[$y, x, -z$]	[7]
8	[$-Y, -X, -Z$]	[$-y, -x, -z$]	[8]
9	[$-X, -Y, -Z$]	[$-x, -y, -z$]	[9]
10	[$X, Y, -Z$]	[$x, y, -z$]	[10]
11	[$Y, -X, -Z$]	[$y, -x, -z$]	[11]
12	[$-Y, X, -Z$]	[$-y, x, -z$]	[12]
13	[$X, -Y, Z$]	[$x, -y, z$]	[13]
14	[$-X, Y, Z$]	[$-x, y, z$]	[14]
15	[$-Y, -X, Z$]	[$-y, -x, z$]	[15]
16	[Y, X, Z]	[y, x, z]	[16]