PG No. 8 D_{2h} mmm [orthorhombic]

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

Table 1: Wyckoff bond: `2a@2a`

No.	vector	center	mapping
1	[0, 0, Z]	[x, 0, 0]	`[1,-4,-6,7]`
2	[0, 0, Z]	[$-x$, 0, 0]	`[2,-3,-5,8]`

Table 2: Wyckoff bond: `2b@2a`

No.	vector	center	mapping
1	[0, Y, 0]	[x, 0, 0]	`[1,-4,6,-7]`
2	[0, $-Y$, 0]	[$-x$, 0, 0]	`[2,-3,5,-8]`

Table 3: Wyckoff bond: `2c@2a`

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

Table 4: Wyckoff bond: `4d@2a`

No.	vector	center	mapping
1	[X, Y, 0]	[x, 0, 0]	`[1,6]`
2	[$-X$, $-Y$, 0]	[$-x$, 0, 0]	`[2,5]`
3	[$-X$, Y, 0]	[$-x$, 0, 0]	`[3,8]`
4	[X, $-Y$, 0]	[x, 0, 0]	`[4,7]`

Table 5: Wyckoff bond: `4e@2a`

No.	vector	center	mapping
1	[X, 0, Z]	[x, 0, 0]	`[1,7]`
2	[$-X$, 0, Z]	[$-x$, 0, 0]	`[2,8]`
3	[$-X$, 0, $-Z$]	[$-x$, 0, 0]	`[3,5]`
4	[X, 0, $-Z$]	[x, 0, 0]	`[4,6]`

Table 6: Wyckoff bond: `4f@2a`

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

Table 7: Wyckoff bond: `8g@2a`

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]`
5	$[-X, -Y, -Z]$	$[-x, 0, 0]$	`[5]`
6	$[X, Y, -Z]$	$[x, 0, 0]$	`[6]`
7	$[X, -Y, Z]$	$[x, 0, 0]$	`[7]`
8	$[-X, Y, Z]$	$[-x, 0, 0]$	`[8]`

* Wyckoff site: `2b`, site symmetry: `m2m`

Table 8: Wyckoff bond: `2a@2b`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, y, 0]$	`[1,-3,-6,8]`
2	$[0, 0, Z]$	$[0, -y, 0]$	`[2,-4,-5,7]`

Table 9: Wyckoff bond: `2b@2b`

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

Table 10: Wyckoff bond: `2c@2b`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, 0]$	`[1,-3,6,-8]`
2	$[-X, 0, 0]$	$[0, -y, 0]$	`[2,-4,5,-7]`

Table 11: Wyckoff bond: `4d@2b`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, y, 0]$	`[1,6]`
2	$[-X, -Y, 0]$	$[0, -y, 0]$	`[2,5]`
3	$[-X, Y, 0]$	$[0, y, 0]$	`[3,8]`
4	$[X, -Y, 0]$	$[0, -y, 0]$	`[4,7]`

Table 12: Wyckoff bond: `4e@2b`

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

Table 13: Wyckoff bond: `4f@2b`

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, 0]$	`[1,8]`
2	$[0, -Y, Z]$	$[0, -y, 0]$	`[2,7]`
3	$[0, Y, -Z]$	$[0, y, 0]$	`[3,6]`
4	$[0, -Y, -Z]$	$[0, -y, 0]$	`[4,5]`

Table 14: Wyckoff bond: `8g@2b`

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]`
5	$[-X, -Y, -Z]$	$[0, -y, 0]$	`[5]`
6	$[X, Y, -Z]$	$[0, y, 0]$	`[6]`
7	$[X, -Y, Z]$	$[0, -y, 0]$	`[7]`
8	$[-X, Y, Z]$	$[0, y, 0]$	`[8]`

* Wyckoff site: `2c`, site symmetry: `mm2`

Table 15: Wyckoff bond: `2a@2c`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,7,8]`
2	$[0, 0, -Z]$	$[0, 0, -z]$	`[3,4,5,6]`

Table 16: Wyckoff bond: `2b@2c`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, z]$	`[1,-2,-7,8]`
2	$[0, Y, 0]$	$[0, 0, -z]$	`[3,-4,-5,6]`

Table 17: Wyckoff bond: `2c@2c`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, z]$	`[1,-2,7,-8]`
2	$[-X, 0, 0]$	$[0, 0, -z]$	`[3,-4,5,-6]`

Table 18: Wyckoff bond: `4d@2c`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	`[1,-2]`
2	$[-X, Y, 0]$	$[0, 0, -z]$	`[3,-4]`
3	$[-X, -Y, 0]$	$[0, 0, -z]$	`[5,-6]`
4	$[X, -Y, 0]$	$[0, 0, z]$	`[7,-8]`

Table 19: Wyckoff bond: `4e@2c`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, z]$	`[1,7]`
2	$[-X, 0, Z]$	$[0, 0, z]$	`[2,8]`
3	$[-X, 0, -Z]$	$[0, 0, -z]$	`[3,5]`
4	$[X, 0, -Z]$	$[0, 0, -z]$	`[4,6]`

Table 20: Wyckoff bond: `4f@2c`

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, z]$	`[1,8]`
2	$[0, -Y, Z]$	$[0, 0, z]$	`[2,7]`
3	$[0, Y, -Z]$	$[0, 0, -z]$	`[3,6]`
4	$[0, -Y, -Z]$	$[0, 0, -z]$	`[4,5]`

Table 21: Wyckoff bond: `8g@2c`

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]`
5	$[-X, -Y, -Z]$	$[0, 0, -z]$	`[5]`
6	$[X, Y, -Z]$	$[0, 0, -z]$	`[6]`
7	$[X, -Y, Z]$	$[0, 0, z]$	`[7]`
8	$[-X, Y, Z]$	$[0, 0, z]$	`[8]`

* Wyckoff site: `4d`, site symmetry: `m..`

Table 22: Wyckoff bond: `4a@4d`

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, z]$	`[1,8]`
2	$[0, -Y, Z]$	$[0, -y, z]$	`[2,7]`
3	$[0, Y, -Z]$	$[0, y, -z]$	`[3,6]`
4	$[0, -Y, -Z]$	$[0, -y, -z]$	`[4,5]`

Table 23: Wyckoff bond: `4b@4d`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	`[1,-8]`
2	$[-X, 0, 0]$	$[0, -y, z]$	`[2,-7]`
3	$[-X, 0, 0]$	$[0, y, -z]$	`[3,-6]`
4	$[X, 0, 0]$	$[0, -y, -z]$	`[4,-5]`

Table 24: Wyckoff bond: `8c@4d`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	`[1]`
2	$[-X, -Y, Z]$	$[0, -y, z]$	`[2]`
3	$[-X, Y, -Z]$	$[0, y, -z]$	`[3]`
4	$[X, -Y, -Z]$	$[0, -y, -z]$	`[4]`
5	$[-X, -Y, -Z]$	$[0, -y, -z]$	`[5]`
6	$[X, Y, -Z]$	$[0, y, -z]$	`[6]`
7	$[X, -Y, Z]$	$[0, -y, z]$	`[7]`
8	$[-X, Y, Z]$	$[0, y, z]$	`[8]`

* Wyckoff site: `4e`, site symmetry: `.m.`

Table 25: Wyckoff bond: `4a@4e`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	`[1,7]`
2	$[-X, 0, Z]$	$[-x, 0, z]$	`[2,8]`
3	$[-X, 0, -Z]$	$[-x, 0, -z]$	`[3,5]`
4	$[X, 0, -Z]$	$[x, 0, -z]$	`[4,6]`

Table 26: Wyckoff bond: `4b@4e`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, z]$	`[1,-7]`
2	$[0, -Y, 0]$	$[-x, 0, z]$	`[2,-8]`
3	$[0, Y, 0]$	$[-x, 0, -z]$	`[3,-5]`
4	$[0, -Y, 0]$	$[x, 0, -z]$	`[4,-6]`

Table 27: Wyckoff bond: `8c@4e`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, z]$	`[1]`
2	$[-X, -Y, Z]$	$[-x, 0, z]$	`[2]`
3	$[-X, Y, -Z]$	$[-x, 0, -z]$	`[3]`
4	$[X, -Y, -Z]$	$[x, 0, -z]$	`[4]`
5	$[-X, -Y, -Z]$	$[-x, 0, -z]$	`[5]`
6	$[X, Y, -Z]$	$[x, 0, -z]$	`[6]`
7	$[X, -Y, Z]$	$[x, 0, z]$	`[7]`
8	$[-X, Y, Z]$	$[-x, 0, z]$	`[8]`

* Wyckoff site: `4f`, site symmetry: `..m`

Table 28: Wyckoff bond: `4a@4f`

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

Table 29: Wyckoff bond: `4b@4f`

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

Table 30: Wyckoff bond: `8c@4f`

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

* Wyckoff site: `8g`, site symmetry: `1`

Table 31: Wyckoff bond: `8a@8g`

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]`
5	$[-X, -Y, -Z]$	$[-x, -y, -z]$	`[5]`
6	$[X, Y, -Z]$	$[x, y, -z]$	`[6]`
7	$[X, -Y, Z]$	$[x, -y, z]$	`[7]`

8	$[-X, Y, Z]$	$[-x, y, z]$	[8]