SG No. 25 C_{2v}^{1} $Pmm2$ [orthorhombic]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `mm2`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,3,4]`

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

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

Table 3: Wyckoff bond: `1c@1a`

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

Table 4: Wyckoff bond: `2d@1a`

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

Table 5: Wyckoff bond: `2e@1a`

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

Table 6: Wyckoff bond: `2f@1a`

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

Table 7: Wyckoff bond: `4g@1a`

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]`

* Wyckoff site: `1b`, site symmetry: `mm2`

Table 8: Wyckoff bond: `1a@1b`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[1,2,3,4]`

Table 9: Wyckoff bond: `1b@1b`

No.	vector	center	mapping
1	$[0, Y, 0]$	$\left[0, \frac{1}{2}, z\right]$	`[1,-2,-3,4]`

Table 10: Wyckoff bond: `1c@1b`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[0, \frac{1}{2}, z\right]$	`[1,-2,3,-4]`

Table 11: Wyckoff bond: `2d@1b`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, \frac{1}{2}, z\right]$	`[1,-2]`
2	$[X, -Y, 0]$	$\left[0, \frac{1}{2}, z\right]$	`[3,-4]`

Table 12: Wyckoff bond: `2e@1b`

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[1,3]`
2	$[-X, 0, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[2,4]`

Table 13: Wyckoff bond: `2f@1b`

No.	vector	center	mapping
1	$[0,\, Y,\, Z]$	$\left[0,\, \frac{1}{2},\, z\right]$	`[1,4]`
2	$[0,\, -Y,\, Z]$	$\left[0,\, \frac{1}{2},\, z\right]$	`[2,3]`

Table 14: Wyckoff bond: `4g@1b`

No.	vector	center	mapping
1	$[X,\, Y,\, Z]$	$\left[0,\, \frac{1}{2},\, z\right]$	`[1]`
2	$[-X,\, -Y,\, Z]$	$\left[0,\, \frac{1}{2},\, z\right]$	`[2]`
3	$[X,\, -Y,\, Z]$	$\left[0,\, \frac{1}{2},\, z\right]$	`[3]`
4	$[-X,\, Y,\, Z]$	$\left[0,\, \frac{1}{2},\, z\right]$	`[4]`

* Wyckoff site: `1c`, site symmetry: `mm2`

Table 15: Wyckoff bond: `1a@1c`

No.	vector	center	mapping
1	$[0,\, 0,\, Z]$	$\left[\frac{1}{2},\, 0,\, z\right]$	`[1,2,3,4]`

Table 16: Wyckoff bond: `1b@1c`

No.	vector	center	mapping
1	$[0,\, Y,\, 0]$	$\left[\frac{1}{2},\, 0,\, z\right]$	`[1,-2,-3,4]`

Table 17: Wyckoff bond: `1c@1c`

No.	vector	center	mapping
1	$[X,\, 0,\, 0]$	$\left[\frac{1}{2},\, 0,\, z\right]$	`[1,-2,3,-4]`

Table 18: Wyckoff bond: `2d@1c`

No.	vector	center	mapping
1	$[X,\, Y,\, 0]$	$\left[\frac{1}{2},\, 0,\, z\right]$	`[1,-2]`
2	$[X,\, -Y,\, 0]$	$\left[\frac{1}{2},\, 0,\, z\right]$	`[3,-4]`

Table 19: Wyckoff bond: `2e@1c`

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[1,3]`
2	$[-X, 0, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[2,4]`

Table 20: Wyckoff bond: `2f@1c`

No.	vector	center	mapping
1	$[0, Y, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[1,4]`
2	$[0, -Y, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[2,3]`

Table 21: Wyckoff bond: `4g@1c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[2]`
3	$[X, -Y, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[3]`
4	$[-X, Y, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[4]`

* Wyckoff site: `1d`, site symmetry: `mm2`

Table 22: Wyckoff bond: `1a@1d`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,2,3,4]`

Table 23: Wyckoff bond: `1b@1d`

No.	vector	center	mapping
1	$[0, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,-2,-3,4]`

Table 24: Wyckoff bond: `1c@1d`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,-2,3,-4]`

Table 25: Wyckoff bond: `2d@1d`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,-2]`
2	$[X, -Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[3,-4]`

Table 26: Wyckoff bond: `2e@1d`

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,3]`
2	$[-X, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[2,4]`

Table 27: Wyckoff bond: `2f@1d`

No.	vector	center	mapping
1	$[0, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,4]`
2	$[0, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[2,3]`

Table 28: Wyckoff bond: `4g@1d`

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

* Wyckoff site: `2e`, site symmetry: `.m.`

Table 29: Wyckoff bond: `2a@2e`

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

Table 30: Wyckoff bond: `2b@2e`

No.	vector	center	mapping
1	$[0,\ Y,\ 0]$	$[x,\ 0,\ z]$	`[1,-3]`
2	$[0,\ -Y,\ 0]$	$[-x,\ 0,\ z]$	`[2,-4]`

Table 31: Wyckoff bond: `4c@2e`

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]`

* Wyckoff site: `2f`, site symmetry: `.m.`

Table 32: Wyckoff bond: `2a@2f`

No.	vector	center	mapping
1	$[X,\ 0,\ Z]$	$\left[x,\ \frac{1}{2},\ z\right]$	`[1,3]`
2	$[-X,\ 0,\ Z]$	$\left[-x,\ \frac{1}{2},\ z\right]$	`[2,4]`

Table 33: Wyckoff bond: `2b@2f`

No.	vector	center	mapping
1	$[0,\ Y,\ 0]$	$\left[x,\ \frac{1}{2},\ z\right]$	`[1,-3]`
2	$[0,\ -Y,\ 0]$	$\left[-x,\ \frac{1}{2},\ z\right]$	`[2,-4]`

Table 34: Wyckoff bond: `4c@2f`

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

* Wyckoff site: `2g`, site symmetry: `m..`

Table 35: Wyckoff bond: `2a@2g`

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

Table 36: Wyckoff bond: `2b@2g`

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

Table 37: Wyckoff bond: `4c@2g`

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]`

* Wyckoff site: `2h`, site symmetry: `m..`

Table 38: Wyckoff bond: `2a@2h`

No.	vector	center	mapping
1	$[0, Y, Z]$	$\left[\frac{1}{2}, y, z\right]$	`[1,4]`
2	$[0, -Y, Z]$	$\left[\frac{1}{2}, -y, z\right]$	`[2,3]`

Table 39: Wyckoff bond: `2b@2h`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[\frac{1}{2}, y, z\right]$	`[1,-4]`
2	$[-X, 0, 0]$	$\left[\frac{1}{2}, -y, z\right]$	`[2,-3]`

Table 40: Wyckoff bond: `4c@2h`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, y, z\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, -y, z\right]$	`[2]`
3	$[X, -Y, Z]$	$\left[\frac{1}{2}, -y, z\right]$	`[3]`
4	$[-X, Y, Z]$	$\left[\frac{1}{2}, y, z\right]$	`[4]`

* Wyckoff site: `4i`, site symmetry: `1`

Table 41: Wyckoff bond: `4a@4i`

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]`