SG No. 127 D_{4h}^{5} $P4/mbm$ [tetragonal]

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

Table 1: Wyckoff site: `2a`, site symmetry: `4/m..`

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4,9,10,11,12]`
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[5,6,7,8,13,14,15,16]`

Table 2: Wyckoff site: `2b`, site symmetry: `4/m..`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,2,3,4,9,10,11,12]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[5,6,7,8,13,14,15,16]`

Table 3: Wyckoff site: `2c`, site symmetry: `m.mm`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,7,8,9,10,15,16]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[3,4,5,6,11,12,13,14]`

Table 4: Wyckoff site: `2d`, site symmetry: `m.mm`

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	`[1,2,7,8,9,10,15,16]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[3,4,5,6,11,12,13,14]`

Table 5: Wyckoff site: `4e`, site symmetry: `4..`

No.	position	mapping
1	$[0, 0, z]$	`[1,2,3,4]`
2	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[5,6,7,8]`
3	$[0, 0, -z]$	`[9,10,11,12]`
4	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[13,14,15,16]`

Table 6: Wyckoff site: `4f`, site symmetry: `2.mm`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,2,15,16]`
2	$\left[\frac{1}{2},\ 0,\ z\right]$	`[3,4,13,14]`
3	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[5,6,11,12]`
4	$\left[0,\ \frac{1}{2},\ -z\right]$	`[7,8,9,10]`

Table 7: Wyckoff site: `4g`, site symmetry: `m.2m`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ 0\right]$	`[1,7,10,16]`
2	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	`[2,8,9,15]`
3	$\left[\frac{1}{2}-x,\ x,\ 0\right]$	`[3,5,12,14]`
4	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	`[4,6,11,13]`

Table 8: Wyckoff site: `4h`, site symmetry: `m.2m`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[1,7,10,16]`
2	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[2,8,9,15]`
3	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}\right]$	`[3,5,12,14]`
4	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[4,6,11,13]`

Table 9: Wyckoff site: `8i`, site symmetry: `m..`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,10]`
2	$[-x,\ -y,\ 0]$	`[2,9]`
3	$[-y,\ x,\ 0]$	`[3,12]`
4	$[y,\ -x,\ 0]$	`[4,11]`
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	`[5,14]`
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[6,13]`
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	`[7,16]`
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ 0\right]$	`[8,15]`

Table 10: Wyckoff site: `8j`, site symmetry: `m..`

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,10]`
2	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[2,9]`
3	$\left[-y,\ x,\ \frac{1}{2}\right]$	`[3,12]`
4	$\left[y,\ -x,\ \frac{1}{2}\right]$	`[4,11]`
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[5,14]`
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[6,13]`
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[7,16]`
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[8,15]`

Table 11: Wyckoff site: `8k`, site symmetry: `..m`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ z\right]$	`[1,16]`
2	$\left[-x,\ \frac{1}{2}-x,\ z\right]$	`[2,15]`
3	$\left[\frac{1}{2}-x,\ x,\ z\right]$	`[3,14]`
4	$\left[x+\frac{1}{2},\ -x,\ z\right]$	`[4,13]`
5	$\left[\frac{1}{2}-x,\ x,\ -z\right]$	`[5,12]`
6	$\left[x+\frac{1}{2},\ -x,\ -z\right]$	`[6,11]`
7	$\left[x,\ x+\frac{1}{2},\ -z\right]$	`[7,10]`
8	$\left[-x,\ \frac{1}{2}-x,\ -z\right]$	`[8,9]`

Table 12: Wyckoff site: `16l`, site symmetry: `1`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1]`
2	$[-x,\ -y,\ z]$	`[2]`
3	$[-y,\ x,\ z]$	`[3]`
4	$[y,\ -x,\ z]$	`[4]`
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	`[5]`
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	`[6]`
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	`[7]`
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ -z\right]$	`[8]`
9	$[-x,\ -y,\ -z]$	`[9]`
10	$[x,\ y,\ -z]$	`[10]`
11	$[y,\ -x,\ -z]$	`[11]`
12	$[-y,\ x,\ -z]$	`[12]`
13	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	`[13]`
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	`[14]`
15	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	`[15]`
16	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	`[16]`