SG No. 125 D_{4h}^3 $P4/nbm$ [tetragonal]

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

Table 1: Wyckoff site: `2a`, site symmetry: `422`

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

Table 2: Wyckoff site: `2b`, site symmetry: `422`

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

Table 3: Wyckoff site: `2c`, site symmetry: `-42m`

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

Table 4: Wyckoff site: `2d`, site symmetry: `-42m`

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

Table 5: Wyckoff site: `4e`, site symmetry: `..2/m`

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `..2`

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

Table 10: Wyckoff site: `8j`, site symmetry: `..2`

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

Table 11: Wyckoff site: `8k`, site symmetry: `.2.`

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

Table 12: Wyckoff site: `8l`, site symmetry: `.2.`

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

Table 13: Wyckoff site: `8m`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ -x,\ z]$	`[1,15]`
2	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ z\right]$	`[2,16]`
3	$\left[x+\frac{1}{2},\ x,\ z\right]$	`[3,13]`

continued ...

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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