SG No. 126 D_{4h}^{4} $P4/nnc$ [tetragonal]

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

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `222.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4..`

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `-1`

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

Table 7: Wyckoff site: `8g`, site symmetry: `2..`

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

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

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

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

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,6]`
2	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[2,5]`
3	$\left[\frac{1}{4},\ x,\ \frac{1}{4}\right]$	`[3,7]`

continued ...

Table 9

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

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

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

Table 11: Wyckoff site: 16k, 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	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[5]
6	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[6]
7	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[7]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[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	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[13]
14	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[14]
15	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[15]
16	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[16]