SG No. 124 D_{4h}^2 $P4/mcc$ [tetragonal]

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

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 422

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

Table 4: Wyckoff site: 2d, site symmetry: 4/m..

No.	position	mapping
1	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	[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 5: Wyckoff site: 4e, site symmetry: 2/m..

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

Table 6: Wyckoff site: `4f`, site symmetry: `222.`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x,\, y,\, 0]$	`[1,10]`
2	$[-x,\, -y,\, 0]$	`[2,9]`
3	$[-y,\, x,\, 0]$	`[3,12]`

continued ...

Table 13

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

Table 14: Wyckoff site: `16n`, 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	$\left[-x,\ y,\ \frac{1}{2}-z\right]$	`[5]`
6	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	`[6]`
7	$\left[y,\ x,\ \frac{1}{2}-z\right]$	`[7]`
8	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	`[8]`
9	$[-x,\ -y,\ -z]$	`[9]`
10	$[x,\ y,\ -z]$	`[10]`
11	$[y,\ -x,\ -z]$	`[11]`
12	$[-y,\ x,\ -z]$	`[12]`
13	$\left[x,\ -y,\ z+\frac{1}{2}\right]$	`[13]`
14	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	`[14]`
15	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	`[15]`
16	$\left[y,\ x,\ z+\frac{1}{2}\right]$	`[16]`