SG No. 131 D_{4h}^{9} $P4_2/mmc$ [tetragonal]

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

Table 1: Wyckoff site: `2a`, site symmetry: `mmm`.

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

Table 2: Wyckoff site: `2b`, site symmetry: `mmm`.

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

Table 3: Wyckoff site: `2c`, site symmetry: `mmm`.

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

Table 4: Wyckoff site: `2d`, site symmetry: `mmm`.

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

Table 5: Wyckoff site: `2e`, site symmetry: `-4m2`

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

Table 6: Wyckoff site: `2f`, site symmetry: `-4m2`

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

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

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

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

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

Table 9: Wyckoff site: `4i`, site symmetry: `2mm.`

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

Table 10: Wyckoff site: `4j`, site symmetry: `m2m.`

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

Table 11: Wyckoff site: `4k`, site symmetry: `m2m.`

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

Table 12: Wyckoff site: `4l`, site symmetry: `m2m.`

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

Table 13: Wyckoff site: `4m`, site symmetry: `m2m.`

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

Table 14: Wyckoff site: `8n`, 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	$\left[-x,\ x,\ \frac{3}{4}\right]$	`[3,5]`
4	$\left[x,\ -x,\ \frac{3}{4}\right]$	`[4,6]`
5	$\left[-x,\ -x,\ \frac{3}{4}\right]$	`[9,15]`
6	$\left[x,\ x,\ \frac{3}{4}\right]$	`[10,16]`
7	$\left[x,\ -x,\ \frac{1}{4}\right]$	`[11,13]`
8	$\left[-x,\ x,\ \frac{1}{4}\right]$	`[12,14]`

Table 15: Wyckoff site: `8o`, site symmetry: `.m.`

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

Table 16: Wyckoff site: `8p`, site symmetry: `.m.`

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

Table 17: Wyckoff site: `8q`, site symmetry: `m..`

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

Table 18: Wyckoff site: `16r`, site symmetry: `1`

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

continued ...

Table 18

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